* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * *				
NEWS	1			Web Page URLs for STN Seminar Schedule - N. America				
NEWS	2			"Ask CAS" for self-help around the clock				
NEWS	3	May	10	PROUSDDR now available on STN				
NEWS	4	May	19	PROUSDDR: One FREE connect hour, per account, in both May				
				and June 2004				
NEWS				EXTEND option available in structure searching				
				Polymer links for the POLYLINK command completed in REGISTRY				
NEWS	7	May	17	FRFULL now available on STN				
NEWS	8	May	27	New UPM (Update Code Maximum) field for more efficient patent				
				SDIs in CAplus				
NEWS								
		-		Explore APOLLIT with free connect time in June 2004				
NEWS	11	Jun	22	STN Patent Forums to be held July 19-22, 2004				
NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004								
NEWS HOURS			STN Operating Hours Plus Help Desk Availability					
NEWS INTER		Gei	General Internet Information					
NEWS LOGIN		We:	Welcome Banner and News Items					
NEWS PHONE		Di	Direct Dial and Telecommunication Network Access to STN					
NEWS WWW CAS World Wide Web Site (general information)								

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter  $\underline{\text{HELP PROP}}$  at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> file casreact COST IN U.S. DOLLARS

SINCE FILE ENTRY SESSION

TOTAL

FULL ESTIMATED COST

10.08 10.29

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT: 1840 - 20 Jun 2004 VOL 140 ISS 25

\*\*\*\*\* CASREACT now has more than 8 million reactions \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

L1STRUCTURE UPLOADED

=> 11

L1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d 11

L1 HAS NO ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 09:44:20 FILE 'CASREACT' SCREENING COMPLETE - 6 REACTIONS TO VERIFY FROM 6 DOCUMENTS

100.0% DONE 6 VERIFIED 0 HIT RXNS SEARCH TIME: 00.00.01

0 DOCS

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH
                                **COMPLETE**
                                 6 TO
PROJECTED VERIFICATIONS:
                                           266
PROJECTED ANSWERS:
                                 0 TO
                                             0
              O SEA SSS SAM L1 ( O REACTIONS)
=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:44:25 FILE 'CASREACT'
                        389 REACTIONS TO VERIFY FROM
                                                        78 DOCUMENTS
SCREENING COMPLETE -
                                                                  0 DOCS
100.0% DONE
              389 VERIFIED
                                  0 HIT RXNS
SEARCH TIME: 00.00.01
              O SEA SSS FUL L1 (
                                   0 REACTIONS)
        STRUCTURE UPLOADED
L4
=> d 14
L4 HAS NO ANSWERS
=> 5 14
SAMPLE SEARCH INITIATED 09:45:43 FILE 'CASREACT'
                         6 REACTIONS TO VERIFY FROM
                                                          6 DOCUMENTS
SCREENING COMPLETE -
                                                                  0 DOCS
               6 VERIFIED
                                  0 HIT RXNS
100.0% DONE
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                        ONLINE **COMPLETE**
                        BATCH
                                **COMPLETE**
                                 6 TO
                                           266
PROJECTED VERIFICATIONS:
                                 0 TO
                                             0
PROJECTED ANSWERS:
              O SEA SSS SAM L4 (
                                    0 REACTIONS)
=> s 14 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:45:48 FILE 'CASREACT'
                       389 REACTIONS TO VERIFY FROM
                                                        78 DOCUMENTS
SCREENING COMPLETE -
                                                                  3 DOCS
                               89 HIT RXNS
100.0% DONE
              389 VERIFIED
SEARCH TIME: 00.00.01
              3 SEA SSS FUL L4 ( 89 REACTIONS)
=> d 16, ibib abs crd, 1-3
     ANSWER 1 OF 3 CASREACT COPYRIGHT 2004 ACS on STN
            Citing
          References
```

6/24/04

139:301299 CASREACT

Structure-Activity Relationships of the p38 $\alpha$  MAP

3-y1) -3-[4-(2-morpholin-4-y1-ethoxy) naph-

Kinase Inhibitor 1-(5-tert-Butyl-2-p-tolyl-2H-pyrazol-

ACCESSION NUMBER:

TITLE:

AUTHOR(S):

SOURCE:

thalen-1-yl]urea (BIRB 796) Regan, John; Capolino, Alison; Cirillo, Pier F.;

Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Kroe, Rachel R.; Madwed, Jeffrey; Moriak, Monica; Nelson, Richard; Pargellis, Christopher A.; Swinamer,

Alan; Torcellini, Carol; Tsang, Michele; Moss, Neil

Department of Medicinal Chemistry, Boehringer

Ingelheim Pharmaceuticals Research and Development

Center, Ridgefield, CT, 06877, USA

Journal of Medicinal Chemistry (2003), 46(22),

4676-4686

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: DOCUMENT TYPE:

CORPORATE SOURCE:

American Chemical Society

LANGUAGE: English

We report on the structure-activity relationships (SAR) of 1-(5-tert-buty1-2-p-toly1-2H-pyrazol-3-y1)-3-[4-(2-morpholin-4-y1ethoxy)naphthalen-1-yl]urea (BIRB 796), an inhibitor of p38α MAP kinase which has advanced into human clin. trials for the treatment of autoimmune diseases. Thermal denaturation was used to establish mol. binding affinities for this class of p38 $\alpha$  inhibitors. The tert-Bu group remains a crit. binding element by occupying a lipophilic domain in the kinase which is exposed upon rearrangement of the activation loop. An arom. ring attached to N-2 of the pyrazole nucleus provides important  $\pi\text{-CH2}$  interactions with the kinase. The role of groups attached through an ethoxy group to the 4-position of the naphthalene and directed into the ATP-binding domain is elucidated. Pharmacophores with good hydrogen bonding potential, such as morpholine, pyridine, and imidazole, shift the melting temp. of  $p38\alpha$  by 16-17° translating into Kd values of 50-100 pM. Finally, we describe several compds. that potently inhibit TNF- $\alpha$  prodn. when dosed orally in mice.

- RX(33) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(34) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(35) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(36) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(37) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(55) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(56) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(57) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(60) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(62) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(63) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(64) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(66) OF 120 REACTION DIAGRAM NOT AVAILABLE
- RX(76) OF 120 REACTION DIAGRAM NOT AVAILABLE

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RX(85) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(86) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(87) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(89) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(90) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(91) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(93) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(94) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(95) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(98) OF 120 - REACTION DIAGRAM NOT AVAILABLE
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RX(102) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(111) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(116) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(117) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(118) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(119) OF 120 - REACTION DIAGRAM NOT AVAILABLE
RX(120) OF 120 - REACTION DIAGRAM NOT AVAILABLE
                              THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                       3.3
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 2 OF 3 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        138:24709 CASREACT
                        Preparation of pyrazole compds. and bis
TITLE:
                        pyrazole-1H-pyrazole intermediates as antiinflammatory
                        agents
                        Kapadia, Suresh R.; Song, Jinhua J.; Yee, Nathan K.
INVENTOR(S):
                        Boehringer Ingelheim Pharmaceuticals, Inc., USA
PATENT ASSIGNEE(S):
                        U.S., 37 pp., Cont.-in-part of U.S. 6,372,773.
SOURCE:
                        CODEN: USXXAM
DOCUMENT TYPE:
                        Patent
                        English
LANGUAGE:
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:
                                     APPLICATION NO. DATE
     PATENT NO.
                 KIND DATE
                                          -----
     ______
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20021210

US 2002-67492

20020205

В1

US 6492529

US 6319921	B1	20011120	US	2000-484638	20000118
US 6333325	B1	20011225	US	2001-871559	20010531
US 6329415	B1	20011211	US	2001-891579	20010626
US 2002065285	A1	20020530	US	2001-891820	20010626
US 6506748	B2	20030114			
US 6372773	B1	20020416	US	2001-920899	20010802
PRIORITY APPLN. INFO.:			US	2000-484638	20000118
			US	2001-920899	20010802
			US	1999-116400P	19990119
			US	2001-891579	20010626
OTHER SOURCE(S):	MA	RPAT 138:24709			

OTHER SOURCE(S):

GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- Pyrazole compds., e.g. I, as well as bis pyrazole-1H-pyrazole intermediate compds. e.q. II, were prepd. The compds. are useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases. All prepd. compds. had IC50 < 10 mM for inhibition of TNF.alpha. in lipopolysaccharide stimulated THP cells.
- RX(74) OF 282 REACTION DIAGRAM NOT AVAILABLE
- RX(79) OF 282 REACTION DIAGRAM NOT AVAILABLE
- RX(82) OF 282 REACTION DIAGRAM NOT AVAILABLE

1. HCl, Dioxane 2. EtN(Pr-i)2, DMSO

RX(84) OF 282 - 2 STEPS

RX(93) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(95) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(96) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(97) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(98) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(105) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(134) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(136) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(141) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(143) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(145) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(147) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(148) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(149) OF 282 - 3 STEPS

1. BrCH2CH2Cl, K2CO3,

2. HCl, Dioxane

3. EtN(Pr-i)2, DMSO

RX(149) OF 282 - 3 STEPS

1. HCl, Dioxane 2. EtN(Pr-i)2, DMSO 3. NaI, Me2CO

# RX(151) OF 282 - 3 STEPS

## RX(152) OF 282 - 4 STEPS

1. BrCH2CH2Cl, K2CO3, MeCN 2. HCl, Dioxane 3. EtN(Pr-i)2, DMSO 4. NaI, Me2CO

RX(152) OF 282 - 4 STEPS

RX(155) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(156) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(164) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(166) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(167) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(168) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(169) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(170) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(175) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(176) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(177) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(178) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(179) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(180) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(181) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(192) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(194) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(230) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(231) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(234) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(235) OF 282 - REACTION DIAGRAM NOT AVAILABLE RX(238) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(239) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(243) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(244) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(245) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(246) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(247) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(251) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(252) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(253) OF 282 - REACTION DIAGRAM NOT AVAILABLE

RX(254) OF 282 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS 5 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## ANSWER 3 OF 3 CASREACT COPYRIGHT 2004 ACS on STN

Citing References

ACCESSION NUMBER:

137:119059 CASREACT TITLE:

Pyrazole Urea-Based Inhibitors of p38 MAP Kinase: From

Lead Compound to Clinical Candidate

AUTHOR (S): Regan, John; Breitfelder, Steffen; Cirillo, Pier;

Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Klaus, Bernhard; Madwed, Jeffrey; Moriak, Monica; Moss, Neil; Pargellis, Chris; Pav, Sue; Proto, Alfred;

Swinamer, Alan; Tong, Liang; Torcellini, Carol

Research and Development Center, Department of CORPORATE SOURCE:

Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA

Journal of Medicinal Chemistry (2002), 45(14), SOURCE:

2994-3008

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal English LANGUAGE:

We report on a series of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase. Importantly, a key binding domain that is distinct from the ATP (ATP) binding site is exposed when the conserved activation loop, consisting in part of Asp168-Phel69-Gly170, adopts a conformation permitting lipophilic and hydrogen bonding interactions between this class of inhibitors and the protein. We describe the correlation of the structure-activity relationships and crystallog. structures of these inhibitors with p38. addn., we incorporated another binding pharmacophore that forms a hydrogen bond at the ATP binding site. This modification affords significant improvements in binding, cellular, and in vivo potencies resulting in the selection of Compd. 45 (BIRB 796) as a clin. candidate for the treatment of inflammatory diseases.

RX(67) OF 99 - REACTION DIAGRAM NOT AVAILABLE

RX(86) OF 99 - REACTION DIAGRAM NOT AVAILABLE

RX(88) OF 99 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 217.25 227.54 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -1.98 -1.98

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

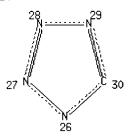
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP CROSSOVER</u> for details.

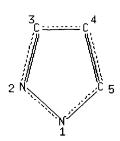
Experimental and calculated property data are now available. For more information enter <a href="https://www.cas.org/online/dbss/registryss.html">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/online/dbss/registryss.html">http://www.cas.org/online/dbss/registryss.html</a>

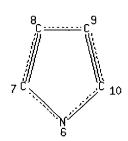
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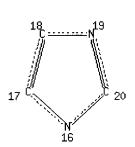
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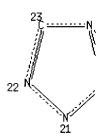


Page 1-A

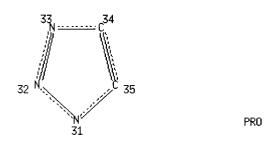


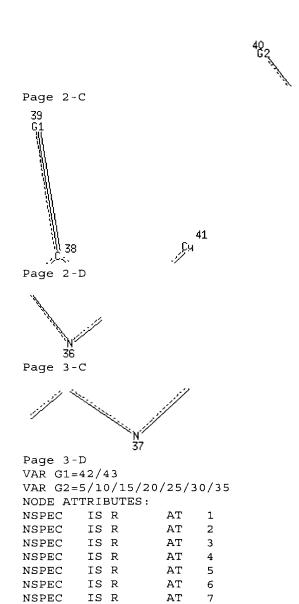






Page 1-D 24 25 Page 1-E





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DEFAULT ECLEVEL IS LIMITED
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#### GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.84	228.38
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.98

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DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

=> s 17/prep

QUALIFICATION NOT VALID FOR L7

Field code qualifications can only be applied to text terms.

=> s 17

SAMPLE SEARCH INITIATED 09:48:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 763 TO ITERATE

100.0% PROCESSED 763 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

13603 TO 16917

PROJECTED ANSWERS:

1081 TO 2159

L8 50 SEA SSS SAM L7

=> s 17 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y FULL SEARCH INITIATED 09:48:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 15438 TO ITERATE

100.0% PROCESSED 15438 ITERATIONS

1575 ANSWERS

50 ANSWERS

SEARCH TIME: 00.00.01

L9 1575 SEA SSS FUL L7

=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

155.42 383.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -1.98

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19/prep

312 L9

3163220 PREP/RL

L10 225 L9/PREP

(L9 (L) PREP/RL)

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 2.36 386.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -1.98

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
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Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by  ${\tt InfoChem}$ .

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

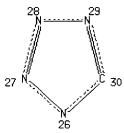
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

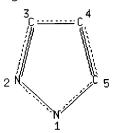
Experimental and calculated property data are now available. For more information enter <a href="https://www.cas.org/ONLINE/DBSS/registryss.html">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

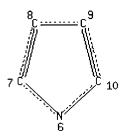
=> L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS L11 STR

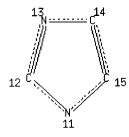


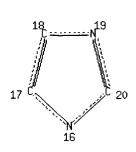
Page 1-A

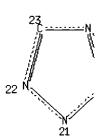




Page 1-C









Page 2-C



NSPEC

Page 3-C VAR G2=5/10/15/20/25/30/35

NODE ATTRIBUTES: NSPEC IS R AT1 2 NSPEC IS R AT3 NSPEC IS R ΑT NSPEC IS R AΤ 4 5 NSPEC IS R ΑT NSPEC 6 IS R ATNSPEC IS R AT7 NSPEC ΑT 8 IS R 9 NSPEC IS R AT10 NSPEC IS R ATNSPEC IS R AT11 NSPEC IS R AT12 NSPEC IS R AΤ 13 NSPEC IS R ΑT 14 NSPEC IS R AT15 NSPEC IS R AT16 NSPEC IS R AT17 NSPEC IS R AT18 NSPEC IS R AT19

IS R

AT

20

50 ANSWERS

```
NSPEC
     IS R
               AT 21
NSPEC IS R
               AT 22
NSPEC IS R
               AT 23
NSPEC IS R
               AT 24
NSPEC IS R
               AT 25
NSPEC IS R
               AT 26
NSPEC IS R
               AT 27
NSPEC IS R
               AT 28
NSPEC IS R
               AT 29
NSPEC IS R
               AT 30
NSPEC IS R
               AT 31
NSPEC IS R
               AT 32
NSPEC IS R
               AΤ
                   33
NSPEC
     IS R
               AΤ
                   34
NSPEC
     IS R
               AT
                   35
NSPEC
      IS C
               AΤ
                   36
NSPEC
      IS C
               AT
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 37
DEFAULT ECLEVEL IS LIMITED
```

### GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

## => s 111

SAMPLE SEARCH INITIATED 09:51:08 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE

3.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: PROJECTED ANSWERS:

559379 TO 579541 117185 TO 126543

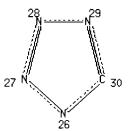
L12 50 SEA SSS SAM L11

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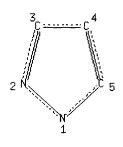
=> d 113

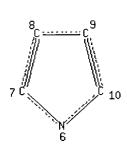
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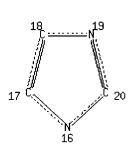
L13 STR

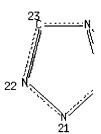


Page 1-A









Page 1-D

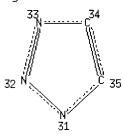
24

25

Page 1-E

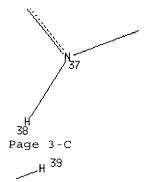
33

34









Page 3-D

		J, 1J, 2U,	23,	30/33
NODE ATT				
NSPEC	IS	R	AT	1
NSPEC	IS		AT	2
NSPEC	IS		AT	3
NSPEC	IS		AT	4
NSPEC	IS		AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12
NSPEC	IS	R	AT	13
NSPEC	IS	R	AT	14
NSPEC	IS	R	AT	15
NSPEC	IS	R	TA	16
NSPEC	IS	R	AT	17
NSPEC	IS	R	ΑT	18
NSPEC	IS	R	ΑT	19
NSPEC	IS	R	AT	20
NSPEC	IS	R	AT	21
NSPEC	IS	R	AT	22
NSPEC	IS	R	ΑT	23
NSPEC	IS	R	AT	24
NSPEC	IS	R	AT	25
NSPEC	IS	R	ΑT	26
NSPEC	IS	R	AT	27
NSPEC	IS	R	AT	28
NSPEC	IS	R	AT	29
NSPEC	IS	R	AT	30
NSPEC	IS	R	AT	31
NSPEC	IS	R	AT	32
NSPEC	IS	R	AT	33
NSPEC	IS	R	ΑT	34
NSPEC	IS	R	ΑT	35
NSPEC	IS	C	ΑT	36
NSPEC	IS	C	AT	37
NSPEC	IS	C	ΑT	38
NSPEC	IS	C	ΑT	39
			_	

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 37 38 39 DEFAULT ECLEVEL IS LIMITED

VAR G2=5/10/15/20/25/30/35

49 ANSWERS

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

=> s 113

SAMPLE SEARCH INITIATED 09:51:58 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE

3.5% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

559379 TO 579541

PROJECTED ANSWERS: 25663 TO 30143

T<sub>1</sub>14

49 SEA SSS SAM L13

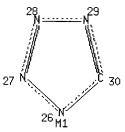
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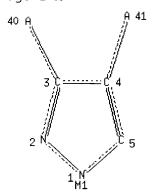
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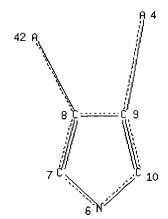
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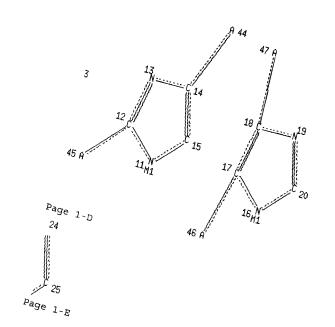
L15 STR

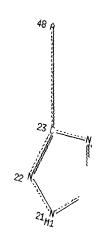


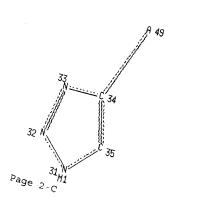
Page 1-A



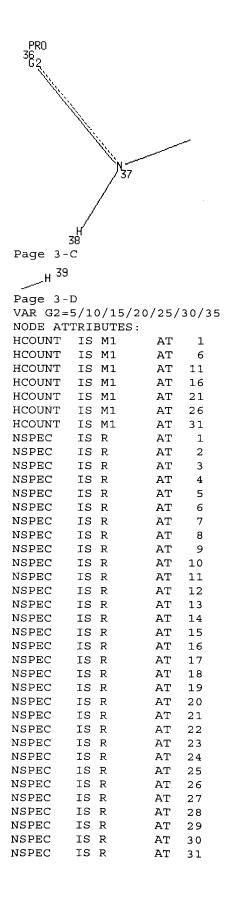








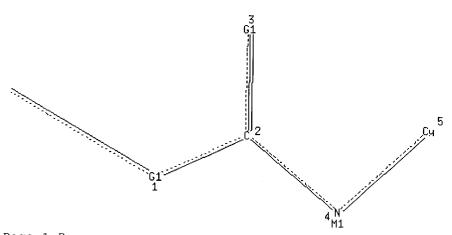
6 M1



```
NSPEC
      IS R
              AT 32
                AT 33
NSPEC IS R
      IS R
                AT
NSPEC
                    34
      IS R
NSPEC
                AT
                    35
NSPEC
      IS C
                AT 36
NSPEC
                AT 37
      IS C
                AT 38
NSPEC IS C
                AT 39
NSPEC IS C
NSPEC IS RC
                AT 40
NSPEC IS RC
                AT 41
NSPEC IS RC
                AT 42
NSPEC IS RC
                AT 43
NSPEC IS RC
                AT 44
NSPEC IS RC
                AT 45
NSPEC IS RC
                AT 46
NSPEC IS RC
                AT 47
NSPEC IS RC
                AT 48
NSPEC IS RC
                AT 49
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 37 38 39 40 41 42 43 44 45 46 47 48 49
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 49
STEREO ATTRIBUTES: NONE
=> s 115
SAMPLE SEARCH INITIATED 09:55:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28473 TO ITERATE
 3.5% PROCESSED
                  1000 ITERATIONS
                                                           8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS:
                      559379 TO 579541
PROJECTED ANSWERS:
                           3650 TO
                                      5460
L16
             8 SEA SSS SAM L15
=>
       STRUCTURE UPLOADED
L17
=> d 117
L17 HAS NO ANSWERS
L17
07 S8
```

6 C.

Page 1-A



```
Page 1-B
VAR G1=7/8
NODE ATTRIBUTES:
HCOUNT IS M1
                AT
NSPEC
      IS C
                AT
NSPEC IS C
                AT
NSPEC IS C
                AT
NSPEC
      IS C
                AT
NSPEC
      IS C
                 AT
NSPEC
       IS RC
                AT
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                     2 4
                           6 7 8
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

=> s 117

SAMPLE SEARCH INITIATED 10:01:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 53469 TO ITERATE

1.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*
BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: PROJECTED ANSWERS:

EXCEEDS 1000000 EXCEEDS 143477

L18 50 SEA SSS SAM L17

=> e indanyl/cn INDANTRIONE/CN E11 E2 1 INDANTRIONE HYDRATE/CN E3 0 --> INDANYL/CN INDANYL (4-(4-(PIPERIDINYL)BUT-1-YNYL)BENZYL)AMINE/CN INDANYL CARBENICILLIN/CN E6 1 INDANYL CARBENICILLIN SODIUM SALT/CN E7 ٦ INDANYL MESYLATE/CN

```
E8
                   INDANYLIUM, 2-((3-ETHOXY-5-METHOXYINDEN-2-YL)METHYLENE)-1-HY
                   DROXY-6-METHOXY-/CN
E9
                   INDANYLPHENOL/CN
             1
E10
                   INDAPAMIDE/CN
             1
E11
             1
                   INDAQUASSIN A/CN
E12
             1
                   INDAQUASSIN B/CN
=> s e7
L19
             1 "INDANYL MESYLATE"/CN
=> d 119
L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
    777-72-0 REGISTRY
    1H-Inden-2-ol, 2,3-dihydro-, methanesulfonate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    2-Indanol, methanesulfonate (7CI, 8CI)
OTHER NAMES:
    2-Indanyl methanesulfonate
     Indanyl mesylate
CN
    NSC 80565
CN
FS
    3D CONCORD
MF
    C10 H12 O3 S
    STN Files:
                 BEILSTEIN*, CA, CAOLD, CAPLUS, PS, TOXCENTER, USPATFULL
         (*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P
      Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent);
      NORL (No role in record)
```

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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10 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
```

```
=> e benzofuran/cn
E1
                   BENZOFUR GG/CN
             1
E2
             1
                   BENZOFUR P/CN
E3
             1 --> BENZOFURAN/CN
E4
             1
                   BENZOFURAN POLYMER/CN
E5
             1
                   BENZOFURAN RADICAL CATION/CN
E6
             1
                   BENZOFURAN, ((2,4-DICHLOROPHENOXY)METHYL)-/CN
F7
             1
                   BENZOFURAN, (2-PROPENYL)-/CN
                   BENZOFURAN, 2 (OR 3) -METHYL-/CN
E8
             1
                   BENZOFURAN, 2,-BIS((P-AMINOPHENYL)ACETYL)-6-METHOXY-/CN
E9
             1
                   BENZOFURAN, 2,2',2'',2'''-(3,6-DIMETHYL-1,2,4,5-BENZENETETRA
E10
             1
                   YL) TETRAKIS-/CN
E11
             1
                   BENZOFURAN, 2,2',2'',2'''-(9,9'-SPIROBI(9H-FLUOREN)-2,2',7,7
                   '-TETRAYL)TETRAKIS-/CN
E12
                   BENZOFURAN, 2,2',2'',2'''- (METHANETETRAYLTETRA-4,1-PHENYLENE
                   ) TETRAKIS-/CN
```

```
=> s e3
L20
             1 BENZOFURAN/CN
=> d 120
L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
     271-89-6 REGISTRY
     Benzofuran (6CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN
     1-Oxindene
CN
     2,3-Benzofuran
CN
     AT 33852
CN
     Benzofurfuran
CN
     Benzo[b] furan
CN
     Coumarone
CN
     NSC 1255
     R 7204
CN
FS
     3D CONCORD
MF
     C8 H6 O
CI
     COM, RPS
LC
     STN Files:
                  AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPLIT,
       ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB,
       IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA,
       PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2,
       USPATFULL, VTB
         (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA
      CAplus document type: Book; Conference; Dissertation; Journal; Patent;
       Preprint; Report
      Roles from patents: ANST (Analytical study); BIOL (Biological study);
RL.P
       FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
      Roles for non-specific derivatives from patents: ANST (Analytical
       study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation);
       PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
       (Uses)
      Roles from non-patents: ANST (Analytical study); BIOL (Biological
       study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
      study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC
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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

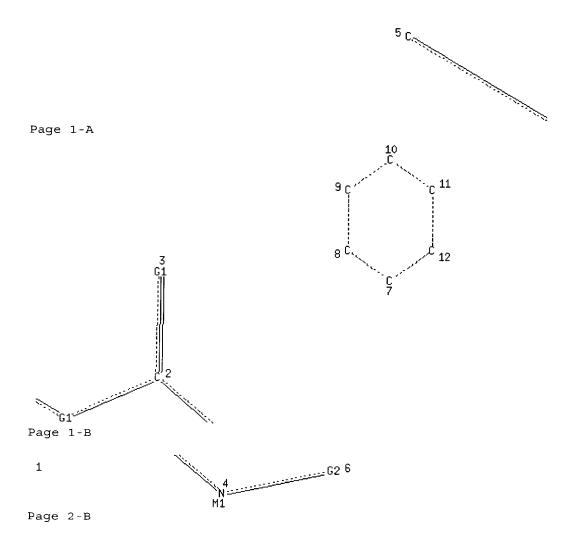
1993 REFERENCES IN FILE CA (1907 TO DATE)
263 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

# 1993 REFERENCES IN FILE CAPLUS (1907 TO DATE) 59 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e indenyl/cn
                         INDENOPYRENE, METHYL-/CN
                        INDENOPYRENONE/CN
E3
                1 --> INDENYL/CN
             1 --> INDENYL/CN
1 INDENYL ANION/CN
1 INDENYL POTASSIUM/CN
1 INDENYL ZIRCONIUM TRIS (DIETHYLCARBAMATE) / CN
1 INDENYL ZIRCONIUM TRIS (TRIMETHYLACETATE) / CN
1 INDENYL (TRI (TERT-BUTYL) PHOSPHINIMIDO) TITANIUM DICHLORIDE / CN
1 INDENYL, 1,2,3,4,5,6,7-HEPTACHLORO-/CN
1 INDENYL, 1-DIOXY-/CN
1 INDENYL, 2-METHYL-/CN
1 INDENYL, 5-HYDROXY-/CN
E5
E6
F.7
E8
E9
E10
E11
E12
=> s e3
L21
                 1 INDENYL/CN
=> d 121
L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
      71551-80-9 REGISTRY
      Indenyl (7CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN
      Inden-2-yl
      2143-54-6, 117988-54-2
DR
MF
     C9 H7
CT
     MAN
LC STN Files: BIOSIS, CA, CAOLD, CAPLUS, TOXCENTER DT.CA CAplus document type: Dissertation; Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); OCCU
         (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
         (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: PREP
         (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or
         reagent)
 STRUCTURE DIAGRAM IS NOT AVAILABLE
                  24 REFERENCES IN FILE CA (1907 TO DATE)
                   4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
                  24 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                    2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
= >
1.22
          STRUCTURE UPLOADED
```

=> d 122

L22 HAS NO ANSWERS



```
15
             17
             18
 14
         13
                     <u>2</u>2
Page 3-B
  20
  21
Page 3-C
VAR G1=23/24
VAR G2 = 7/20
NODE ATTRIBUTES:
HCOUNT
        IS M1
                    AT
NSPEC
         IS C
                    AT
NSPEC
         IS C
                    AT
NSPEC
         IS C
                    ΑT
         IS C
NSPEC
                    AT
NSPEC
         IS RC
                    AT
NSPEC
         IS C
                    AT
                         6
NSPEC
         IS R
                    AT
                         7
NSPEC
         IS R
                    AT
                         8
NSPEC
         IS R
                    AT
                         9
NSPEC
         IS R
                    AT
                        10
NSPEC
        IS R
                    AT
                        11
NSPEC
        IS R
                    AT
                        12
NSPEC
        IS R
                    AT
                        13
NSPEC
        IS R
                    ΑТ
                        14
NSPEC
        IS R
                    AΤ
                        15
NSPEC
        IS R
                    AT
                        16
NSPEC
        IS R
                    ΑT
                        17
NSPEC
        IS R
                    TA
                        18
NSPEC
         IS R
                    AT
                        19
NSPEC
         IS R
                    AT
                        20
NSPEC
        IS R
                    AT
                        21
NSPEC
        IS R
                   AΤ
                        22
DEFAULT MLEVEL IS ATOM
MLEVEL
        IS CLASS AT
                         2
                                5 23 24
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
```

=> s 122

SAMPLE SEARCH INITIATED 10:10:45 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 12830 TO ITERATE

7.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

249817 TO 263383

PROJECTED ANSWERS:

62503 TO 69389

50 SEA SSS SAM L22

=> s 122 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y FULL SEARCH INITIATED 10:10:51 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 259836 TO ITERATE

100.0% PROCESSED 259836 ITERATIONS

65845 ANSWERS

SEARCH TIME: 00.00.02

65845 SEA SSS FUL L22 T.24

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 189.14 575.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY

SESSION CA SUBSCRIBER PRICE 0.00 -1.98

FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 124/rct

26409 L24

2633407 RCT/RL

6528 L24/RCT

(L24 (L) RCT/RL)

```
=> d his
     (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
     FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
     FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
Ll
                STRUCTURE UPLOADED
L2
              0 S L1
L3
              0 S L1 FULL
                STRUCTURE UPLOADED
L4
              0 S L4
L5
              3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7
                STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
             50 S L7
L8
           1575 S L7 FULL
L9
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
T.10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                STRUCTURE UPLOADED
L12
             50 S L11
L13
                STRUCTURE UPLOADED
             49 S L13
L14
                STRUCTURE UPLOADED
L15
L16
             8 S L15
L17
                STRUCTURE UPLOADED
L18
             50 S L17
                E INDANYL/CN
              1 S E7
L19
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
L21
              1 S E3
                STRUCTURE UPLOADED
L22
L23
             50 S L22
          65845 S L22 FULL
    FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
          6528 S L24/RCT
=> s 125 and 110
            21 L25 AND L10
=> file reg
COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                 TOTAL
                                                       ENTRY
                                                              SESSION
FULL ESTIMATED COST
                                                        9.44
                                                                584.74
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                 SINCE FILE
                                                                 TOTAL
                                                       ENTRY
                                                                SESSION
CA SUBSCRIBER PRICE
                                                        0.00
                                                                 -1.98
FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
```

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

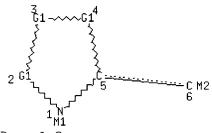
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <a href="https://www.cas.org/ONLINE/DBSS/registryss.html">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> L27 STRUCTURE UPLOADED

=> d 127 L27 HAS NO ANSWERS L27 STE

C 7 N 8 Page 1-A



Page 1-B VAR G1=7/8

NODE ATTRIBUTES:

HCOUNT IS M1 AT7 HCOUNT IS M2 ΑТ IS R AΤ NSPEC 1 NSPEC IS R AΤ 2 NSPEC IS R TA3 NSPEC IS R AΤ 4 NSPEC IS R AT IS C NSPEC ΑT

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 6

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

=> s 127 SAMPLE SEARCH INITIATED 10:13:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 244417 TO ITERATE

1000 ITERATIONS 0.4% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) 50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS:

EXCEEDS 1000000

PROJECTED ANSWERS:

EXCEEDS 329523

50 SEA SSS SAM L27 T.2.8

=> file hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION 0.42 585.16 585.16

FULL ESTIMATED COST

0.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY

SESSION -1.98 0.00

CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

STRUCTURE UPLOADED L1

0 S L1 L2

0 S L1 FULL L3

STRUCTURE UPLOADED L4

```
L5
               0 S L4
L6
              3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
1.7
                STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
Ъ8
             50 S L7
           1575 S L7 FULL
L9
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
                STRUCTURE UPLOADED
L11
             50 S L11
L12
L13
                STRUCTURE UPLOADED
L14
             49 S L13
L15
                STRUCTURE UPLOADED
L16
              8 S L15
L17
                STRUCTURE UPLOADED
             50 S L17
L18
                E INDANYL/CN
              1 S E7
L19
                E BENZOFURAN/CN
              1 S E3
L20
                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                STRUCTURE UPLOADED
             50 S L27
L28
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
=> s 126 and tan, z?/au
          1089 TAN, Z?/AU
L29
             0 L26 AND TAN, Z?/AU
=> s 126 and song, j?/au
          4843 SONG, J?/AU
             0 L26 AND SONG, J?/AU
L30
=> d 126, ibib abs hitstr, 1-21
L26 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
   Full
          Citing
         References
   Text
ACCESSION NUMBER:
                         2004:60480 HCAPLUS
DOCUMENT NUMBER:
                         140:111415
TITLE:
                         Preparation of imidazole derivatives as chymase
                         inhibitors
INVENTOR(S):
                         Kitano, Masafumi; Yamaguchi, Hiroki
```

PATENT ASSIGNEE(S):

Sumitomo Pharmaceuticals Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 122 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO. KI					DATE			A	PPLI	CATI	N NC	Э.	DATE				
									-	<b></b>				<del>-</del>				
WO	2004	0074	64	Α	1	2004	0122		W	0 20	03-J	P868	2	2003	0708			
	W: AE, AG, AL,					ΑT,	AU,	AZ,	ВA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	KΖ,	LC,	LK,	LR,	LS,	
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	PG,	
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,	TR,	
		TT,	TZ,	UA,	ŪG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	
		KZ,	MD,	RŲ,	TJ													
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	BG,	
		CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	
		ΝL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	
		GW,	ML,	MR,	NE,	SN,	TD,	TG										
PRIORITY					JP 2	002-	2017	39	Α	2002	0710							
OTHER SO		MARPAT 140:111415																
GI																		

The title compds. I [wherein X1 = (un)substituted alkylene; X2 and Q = independently a single bond or (un)substituted alkylene; Y1 = (hetero)cyclylene; Y2 = (hetero)cyclyl; M = (un)substituted CO2H, SO3H, CONH2, SO2NH2, -NHSO2H, or tetrazolyl, etc.; R1 and R2 = independently (hetero)cyclyl, H, halo, NO2, CN, CO2H, (un)substituted alkyl, alkenyl, alkynyl, alkoxycarbonyl, acyl, OH, NH2, CONH2, SO2NH2, SH, SOH, or SO2H, etc.] or prodrugs, or pharmaceutically acceptable salts thereof are prepd. For example, the compd. II was prepd. in a multi-step synthesis. II showed inhibitory activity with IC50 of 0.026 µM against human chymase. I have chymase inhibitory activity, and are useful as a therapeutic agent for hypertension, cardiac failure, etc. (no data).

IT 647850-05-3P 647850-07-5P

RN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of imidazole derivs. as chymase inhibitors) 647850-05-3 HCAPLUS

CN Benzoic acid, 2-[[[[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 647850-07-5 HCAPLUS

CN Benzoic acid, 2-[[[methyl[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 259537-23-0P 439142-85-5P 647850-99-5P

647851-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of imidazole derivs. as chymase inhibitors)

RN <u>259537-23-0</u> HCAPLUS

CN Benzoic acid, 2-[(phenoxycarbonyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 439142-85-5 HCAPLUS

CN Carbamic acid, [2-(4-morpholinylcarbonyl)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>647850-99-5</u> HCAPLUS CN Morpholine, 4-[2-[[[

Morpholine, 4-[2-[[[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

RN <u>647851-03-4</u> HCAPLUS

CN Benzoic acid, 2-[[[methyl[1-(1-naphthalenylmethyl)-1H-imidazol-2-yl]amino]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

8

Full Citing Text References

ACCESSION NUMBER:

2004:41269 HCAPLUS

DOCUMENT NUMBER:

140:77038

TITLE:

Preparation of 3-[heteroarylmethoxy]pyridines and

their analogues as p38 map kinase inhibitors

INVENTOR(S):

Murray, Christopher William; Hartshorn, Michael John; Frederickson, Martyn; Congreve, Miles Stuart; Padova, Alessandro; Woodhead, Steven John; Gill, Adrian Liam;

Woodhead, Andrew James

PATENT ASSIGNEE(S):

Astex Technology Limited, UK

SOURCE:

PCT Int. Appl., 134 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA:	CENT	NO.		KIND DATE			APPLICATION NO. DATE										
	<b></b>						- <b>-</b>		_								
WO	2004	0047	2.0	A1 20040115					W	20	03-G	3286	4	2003	0703		
W: AE, AG,			AI.	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
	•••	CO	CR.	CU.	CZ.	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM	HR.	HII.	TD.	IL.	IN.	ıs,	JP,	KE,	KG,	KΡ,	KR,	KΖ,	LC,	LK,	LR,
		LS.	I.T	LII.	LV.	MA.	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NI,	NO,	NZ,	OM,
		PG	DH,	PT.	PT.	RO,	RU.	sc.	SD,	SE,	SG,	sĸ,	SL,	SY,	ТJ,	TM,	TN,
		TR.	TT.	TZ.	UA,	ŪĠ,	US,	υZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,

```
KG, KZ, MD, RU
                     RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
                               GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:
                                                                                               GB 2002-15383
                                                                                                                                              20020703
                                                                                                                                       A
                                                                                               US 2002-393121P P
                                                                                                                                              20020703
                                                                                               GB 2002-26149
                                                                                                                                     A 20021108
OTHER SOURCE(S):
                                                          MARPAT 140:77038
GΙ
           Title compds. I [X=Y = CR2=CR3, CR2=N; R1 = H, halo, amino, etc.; R2-3 =
           H, alkyl, aryl, etc.; R4 = carboaryl, heteroaryl; R5 = halo, amino,
           carboxamido, etc.] are prepd. For instance, 2-amino-3-benzyloxypyridine
           is prepd. by alkylation of 2-amino-3-hydroxypyridine with benzyl chloride.
           A related example, 2-amino-3-[2-phenylbenzyloxy]pyridine has IC50 <
           10\mu M for p38 map kinase. I are useful in the treatment of diseases
           ameliorated by inhibiting p38 MAP kinase.
IT 642084-55-7P, 2-[2-Fluoro-5-[[[[1-(tert-butyl)-3-phenylpyrazol-5-
           yl]amino]carbonyl]amino]benzyloxy]pyrazine 642085-05-0P,
           yl)oxy)methyl)phenyl]urea 642085-37-8P, N-(5-tert-Butyl-2-phenyl-
           {\tt 2H-pyrazol-3-yl)-N'-[4-fluoro-3-(((pyrazin-2-yl)oxy)methyl)phenyl]} ure a the property of the property of
           642085-49-2P, N-[5-tert-Butyl-2-(2,4-difluorophenyl)-2H-pyrazol-3-
           yl]-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea 642085-50-5P
           N-[5-tert-Butyl-2-(4-chlorophenyl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-
           (pyrazin-2-yloxymethyl)phenyl]urea 642085-51-6P,
           N-[5-(4-Chlorophenyl)-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazin-2-phenyl-2H-pyrazin-2-phenyl-2H-pyrazin-2-phenyl-2H-pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl-2-phenyl
           yloxymethyl)phenyl]urea 642085-52-7P, N-(5-tert-Butyl-2-p-tolyl-
           2H-pyrazol-3-yl)-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea
           642085-53-8P, N-[5-(4-Chlorophenyl)-2-(4-fluorophenyl)-2H-pyrazol-
           3-yl]-N'-[4-fluoro-3-(pyrazin-2-yloxymethyl)phenyl]urea
           642085-54-9P, N-(2,5-Diphenyl-2H-pyrazol-3-yl)-N'-[4-fluoro-3-
           (pyrazin-2-yloxymethyl)phenyl]urea 642085-56-1P,
          N-(2-Benzyl-5-tert-butyl-2H-pyrazol-3-yl)-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-57-2P, N-(2-(Benzothiazol-2-yl)-5-
           (tert-butyl)-2H-pyrazol-3-yl)-N'-[4-fluoro-3-(((pyrazin-2-
          yl)oxy)methyl)phenyl]urea 642085-58-3P, N-[5-tert-Butyl-2-(6-
          chloropyridazin-3-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-59-4P, N-[5-tert-Butyl-2-(2,6-
          dimethylpyrimidin-4-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea \underline{642085-61-8P}, N-(5-(tert-Butyl)-2-
           (pyridin-4-yl) -2H-pyrazol-3-yl) -N'- [4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-62-9P, N-[2-(4-Fluorophenyl)-5-
           (tetrahydrofuran-2-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-63-0P, N-[5-(tert-Butyl)-2-(4-
          (methanesulfonyl)phenyl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-64-1P, N-[2-(4-tert-Butylphenyl)-
          5-cyclopropyl-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          yloxymethyl)phenyl]urea 642085-65-2P, N-[2-(4-Fluorophenyl)-5-
          (tetrahydropyran-4-yl)-2H-pyrazol-3-yl]-N'-[4-fluoro-3-(pyrazin-2-
          vloxymethyl)phenyl]urea
          RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
          (Therapeutic use); BIOL (Biological study); PREP (Preparation);
```

USES (Uses)

CN

(prepn. of 3-[heteroarylmethoxy]pyridines and their analogs as p38 map kinase inhibitors for treatment of arthritis)

RN 642084-55-7 HCAPLUS

Urea, N-[1-(1,1-dimethylethyl)-3-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-05-0 HCAPLUS

CN Urea, N-[4-chloro-3-[(3-pyridinyloxy)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-phenyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 642085-37-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-49-2 HCAPLUS

CN Urea, N-[1-(2,4-difluorophenyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-50-5 HCAPLUS

CN Urea, N-[1-(4-chlorophenyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-51-6 HCAPLUS

CN Urea, N-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN <u>642085-52-7</u> HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-53-8 HCAPLUS

CN Urea, N-[3-(4-chlorophenyl)-1-(4-fluorophenyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-54-9 HCAPLUS

Urea, N-(1,3-diphenyl-1H-pyrazol-5-yl)-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-56-1 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(phenylmethyl)-1H-pyrazol-5-yl]-N'-[4-CNfluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-57-2 HCAPLUS

Urea, N-[1-(2-benzothiazolyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-CN fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN642085-58-3 HCAPLUS

CNUrea, N-[1-(6-chloro-3-pyridazinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]- N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-59-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,6-dimethyl-4-pyrimidinyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{NH} \\ -\text{C-NH} \\ -\text{CH} \\ 2-\text{O} \\ \text{N} \\ \text{N} \\ \end{array}$$

RN 642085-61-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-pyridinyl)-1H-pyrazol-5-yl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & & \\ N & & \\ O-CH_2 & & \\ \hline \end{array}$$
 
$$\begin{array}{c|c} N & & \\ NH-C-NH & & \\ \hline \end{array}$$
 
$$\begin{array}{c|c} N & & \\ N & & \\ \hline \end{array}$$

RN 642085-62-9 HCAPLUS

CN Urea, N-[1-(4-fluorophenyl)-3-(tetrahydro-2-furanyl)-1H-pyrazol-5-yl]-N'[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-63-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-[4-(methylsulfonyl)phenyl]-1H-pyrazol-5-CNyl]-N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-64-1 HCAPLUS

Urea, N-[3-cyclopropyl-1-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-5-yl]-N'-CN[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 642085-65-2 HCAPLUS

Urea, N-[1-(4-fluorophenyl)-3-(tetrahydro-2H-pyran-4-yl)-1H-pyrazol-5-yl]-CN N'-[4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]- (9CI) (CA INDEX NAME)

IT 642085-13-0P, (4-Fluoro-3-hydroxymethylphenyl)carbamic acid

tert-butyl ester **642085-14-1P**, [4-Fluoro-3-(((pyrazin-2-

yl)oxy)methyl)phenyl]carbamic acid tert-butyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of 3-[heteroarylmethoxy]pyridines and their analogs as p38 map kinase inhibitors for treatment of arthritis)

642085-13-0 HCAPLUS RN

CN Carbamic acid, [4-fluoro-3-(hydroxymethyl)phenyl]-, 1,1-dimethylethyl
 ester (9CI) (CA INDEX NAME)

RN 642085-14-1 HCAPLUS

CN Carbamic acid, [4-fluoro-3-[(pyrazinyloxy)methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

139:395938

## Full Citing Text References

ACCESSION NUMBER:

2003:892762 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Preparation of ureas as positive allosteric modulators

of the nicotinic acetylcholine receptor

INVENTOR(S):

Piotrowski, David W.; Rogers, Bruce N.; McWhorter, William W., Jr.; Walker, Daniel P.; Corbett, Jeffrey

W.; Groppi, Vincent E., Jr.; Rudmann, Daniel G.

PATENT ASSIGNEE(S): SOURCE:

Pharmacia & Upjohn Company, USA PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.			KI	ND 1	DATE			A.	PPLI	CATIO	N NC	o. 1	DATE				
						<b>-</b> -	<b></b> -		_									
	WO 2003	0932	50	A	2 2	2003	1113		W	20	03-U	S114	93	2003	0428			
W: AE, AG,			AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	OM,	PH,	
		PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,	
		UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	KΖ,	MD,	
		RU,	ΤJ,	TM														
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	BG,	
		CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	
		NL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	

GW, ML, MR, NE, SN, TD, TG

<u>US 2003236287</u> A1 20031225 <u>US 2003-423062</u> 20030425 PRIORITY APPLN. INFO.: <u>US 2002-377364P</u> P 20020503 <u>US 2003-456941P</u> P 20030324

OTHER SOURCE(S): MARPAT 139:395938

AB ANHCXNHB [X = 0, S; A = (un)substituted Ph, 6-membered N heteroaryl; B = (un)substituted 5-6-membered heteroaryl] were prepd. to treat diseases or conditions in which the  $\alpha$ 7 nAChR is known to be involved (no data). Thus, 2,4-Me (MeO) C6H3NH2 was treated with 3-F3CC6H4CNO to give 2,4-Me (MeO) C6H3NHCONHC6H4CF3-3.

IT 553661-25-9P 625120-00-5P 625120-03-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of ureas as pos. allosteric modulators of the nicotinic acetylcholine receptor)

RN 553661-25-9 HCAPLUS

CN Carbamic acid, [3-(trifluoromethoxy)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 625120-00-5 HCAPLUS

CN Carbamic acid, [4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylphenyl], phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \text{PhO} - C - \text{NH} \\ \text{Me} \\ \text{t-Bu} - \text{Si} - 0 \\ \text{Me} \end{array}$$

RN 625120-03-8 HCAPLUS

CN Carbamic acid, (5-chloro-2,4-dimethoxyphenyl)-, phenyl ester (9CI) (CA INDEX NAME)

IT 625117-68-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of ureas as pos. allosteric modulators of the nicotinic

acetylcholine receptor)

RN 625117-68-2 HCAPLUS

CN Urea, N-(5-chloro-2,4-dimethoxyphenyl)-N'-1H-imidazol-2-yl- (9CI) (CA INDEX NAME)

HCAPLUS COPYRIGHT 2004 ACS on STN L26 ANSWER 4 OF 21

139:86541

Citing References

ACCESSION NUMBER:

2003:508521 HCAPLUS

DOCUMENT NUMBER:

TITLE:

N-containing heterocycle stable free radicals and

rubber compositions containing them

INVENTOR(S):

Tomono, Keisuke; Miyashita, Naoshi; Shimada, Atsushi Yokohama Rubber Co., Ltd., Japan

PATENT ASSIGNEE(S):

SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE \_\_\_\_\_ \_\_\_\_\_ \_\_\_\_\_ JP 2003183276 20030703 JP 2001-380398 20011213 A2 JP 2001-380398 20011213 PRIORITY APPLN. INFO .:

OTHER SOURCE(S):

MARPAT 139:86541

The radicals, which are stable at room temp. in the presence of O, have AB N-contg. heterocycles and ≥1 hydrogen bond-formable bonds chosen from (thio)urethane, (thio)urea, (thio)amide, (thio)ester, and ether. Thus, a test piece comprising vulcanized product of a compn. comprising RSS 1 (natural rubber) 100, I (manufd. from 2,4-TDI, 4-hydroxy-2,2,6,6tetramethylpiperidine-1-oxyl, and 3-hydroxy-1,2,4-triazole) 0.1, HAF Shoblack N 339 (carbon black) 50, ZnO 3, sulfur 2, and other additives showed  $tan\delta$  0.1138 at 100°.

IT 552885-92-4P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use);

PREP (Preparation); USES (Uses)

(N-contg. heterocycle stable free radicals as heat-stabilizers for rubber compns. with good vibration damping property)

I

RN552885-92-4 HCAPLUS

1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[[[2(or 4)-methyl-5-[[(1H-1,2,4triazol-3-ylamino)carbonyl]amino]phenyl]amino]carbonyl]oxy]- (9CI) (CA INDEX NAME)

D1-Me

IT 376590-90-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP

(Preparation); RACT (Reactant or reagent)

(N-contg. heterocycle stable free radicals as heat-stabilizers for rubber compns. with good vibration damping property)

RN 376590-90-8 HCAPLUS

CN 1-Piperidinyloxy, 4-[[[[3(or 5)-isocyanato-4(or 2)-

methylphenyl]amino]carbonyl]oxy]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

D1-Me

L26 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Text References
ACCESSION NUMBER:

2002:428885 HCAPLUS

DOCUMENT NUMBER:

NUMBER: 137:6179

TITLE:

Preparation of benzimidazoles as TIE-2 and/or VEGFR2

inhibitors

INVENTOR(S):

Cheung, Mui; Harris, Philip Anthony; Hasegawa, Masaichi; Ida, Satoru; Kano, Kazuya; Nishigaki,

Naohiko; Sato, Hideyuki; Veal, James Martin; Washio,

Yoshiaki; West, Rob I.

PATENT ASSIGNEE(S):

Glaxo Group Limited, UK; Glaxosmithkline K.K.

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.				ND	DATE			А	PPLI	CATI	ON N	0.	DATE					
									_										
WO	WO 2002044156				2	20020606			W	0 20	01-U	S445	53	2001	1128				
WO	WO 2002044156			Α	3	2002	1017												
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	ВG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,		
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,		
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	ΤZ,	UA,		
		UG,	US,	UΖ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,		

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CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                                               20011128
                                            AU 2002-32439
     AU 2002032439
                       Α5
                             20020611
                             20030910
                                             EP 2001-991963
                                                               20011128
     EP 1341771
                        A2
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                             JP 2002-546526
                                                               20011128
     JP 2004517080
                             20040610
                        T2
     US 2004082583
                        Α1
                             20040429
                                             US 2003-433128
                                                               20031112
                                          US 2000-253868P P
US 2001-310939P P
                                                               20001129
PRIORITY APPLN. INFO.:
                                                               20010808
                                          WO 2001-US44553
                                                           W
                                                               20011128
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OTHER SOURCE(S):

MARPAT 137:6179

The title compds. [I; E = (un) substituted aryl, heteroaryl; A = aryl, AB heteroaryl, heterocyclyl; X = S, O, SO2, SO, CH2, CHOH, CO; Z = O, S; P = O0-1; q = 0-1; D = CH, T = CR8, M = C and Q = NT7p, wherein p = 0 and q = 01; or D = CH, T = CR8, M = C and Q = NR7p, wherein p = 1 and q = 0, or D = 1CH, T = CR8, M = C and Q = S or O, wherein q = 0; or D = N, T = CR8, M = Cand Q = NR7p, wherein either p or q = 0 and the other = 1; or D = CH, T =N, M = C and Q = NR7p, wherein either p or q = 0 and the other = 1; or D = 0CH, T = CR8, M = N and Q = CH, wherein q = 0; R1 = alkyl, haloalkyl, aryl, etc.; R2 = H, alkyl, aryl, etc.; R3 = alkylene or alkylene substituted by oxo, and is linked together with N atom to which it is attached and to one of the benzimidazole N atoms to form a heterocyclic compd. fused to the benzimidazole; R7 = H, alkyl, etc.; R8 = H, halo] and their salts, useful in the treatment of hyperproliferative diseases, were prepd. Thus, reacting Me [5-(4-aminophenoxy)-1H-benzimidazol-2-yl]carbamate (prepn. given) with 3-chlorophenyl isocyanate in THF afforded 69% II which showed pIC50 of > 7.0 in TIE-2 and VEGFR2 enzyme assays.

Π

IT 433225-52-6P 433225-66-2P 433225-79-7P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

RN433225-52-6 HCAPLUS

CN

Acetamide, N-[5-[4-[[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3yl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 433225-66-2 HCAPLUS

CN Acetamide, 2-(2-methoxyethoxy)-N-[5-[4-[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3-yl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-B

-- CH 2-- CH 2-- OMe

RN 433225-79-7 HCAPLUS

CN 2-Furancarboxamide, N-[5-[4-[[[5-(4-morpholinyl)-1H-1,2,4-triazol-3-yl]amino]carbonyl]amino]phenoxy]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

IT 433225-36-6P 433225-37-7P 433225-38-8P

433225-86-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

RN 433225-36-6 HCAPLUS

CN Urea, N-[2-fluoro-5-(trifluoromethyl)phenyl]-N'-[4-[[2-[[[[2-fluoro-5-(trifluoromethyl)phenyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]- (9CI) (CA INDEX NAME)

RN 433225-37-7 HCAPLUS

CN Urea, N-[4-[[2-[[[(4-chlorophenyl)amino]carbonyl]amino]-1H-benzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX

NAME)

433225-38-8 HCAPLUS RN Urea, N-[4-[[2-[[[4-(dimethylamino)phenyl]amino]carbonyl]amino]-1H-CNbenzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

433225-86-6 HCAPLUS RN Urea, N-[4-[[2-[[(2,3-dimethylphenyl)amino]carbonyl]amino]-1H-CN benzimidazol-5-yl]oxy]phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

IT 54840-15-2, 4-(tert-Butoxycarbonyl)aminophenol 433226-40-5 RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors) 54840-15-2 HCAPLUS RN

Carbamic acid, (4-hydroxyphenyl)-, 1,1-dimethylethyl ester (9CI) (CA CN INDEX NAME)

433226-40-5 HCAPLUS RN

Carbamic acid, [6-[4-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-1H-CN imidazo[4,5-b]pyridin-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

IT 433226-08-5P, 2-Nitro-5-(4-(tert-butoxycarbonylamino)phenoxy)pyrid in-3-ylamine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazoles as TIE-2 and/or VEGFR2 inhibitors)

RN 433226-08-5 HCAPLUS

Carbamic acid, [4-[(5-amino-6-nitro-3-pyridinyl)oxy]phenyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L26 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

INVENTOR(S):

2002:314913 HCAPLUS

136:340689

Preparation of urea derivatives containing nitrogenous aromatic ring compounds as inhibitors of angiogenesis Funahashi, Yasuhiro; Tsuruoka, Akihiko; Matsukura, Masayuki; Haneda, Toru; Fukuda, Yoshio; Kamata, Junichi; Takahashi, Keiko; Matsushima, Tomohiro; Miyazaki, Kazuki; Nomoto, Kenichi; Watanabe, Tatsuo; Obaishi, Hiroshi; Yamaguchi, Atsumi; Suzuki, Sachi; Nakamura, Katsuji; Mimura, Fusayo; Yamamoto, Yuji; Matsui, Junji; Matsui, Kenji; Yoshiba, Takako; Suzuki,

PATENT ASSIGNEE(S):

Yasuyuki; Arimoto, Itaru Eisai Co., Ltd., Japan PCT Int. Appl., 699 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

SOURCE:

Patent Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KINI						DATE			APPLICATION NO. DATE									
LATE				10.11		D2111			71.		CHIL	014 14	J.	DAIL				
									-									
WO 2002032872 A1					1	2002	0425		WO 2001-JP9221 20011019									
WO 2002032872 C1					1	2002	0926											
W	:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PH,	PL,	
		PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	
		US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM		
R'	W:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZW,	AT,	BE,	CH,	CY,	
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
AU 20	AU 2001095986					A5 20020429					AU 2001-95986 20011019							

EP 1415987 A1 20040506 EP 2001-976786 20011019 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR NO 2003001731 A1 20030619 Α NO 2003-1731 20030414 US 2004053908 20040318 US 2003-420466 20030418 

 JP
 2000-320420
 A
 20001020

 JP
 2000-386195
 A
 20001220

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 2001-46685
 A
 20010222

 WO
 2001-JP9221
 W
 20011019

 PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARPAT 136:340689 GI

N-aryl or N-heteroarylurea derivs. represented by the general formula AB Ag-Xg-Yg-Tgl or salts thereof, or hydrates of both [wherein Aq = (un) substituted C6-14 aryl or 5- to 14-membered heterocyclic group; Xg = single bond, O, S, C1-6 alkylene, SO, SO2, (un) substituted NH; Yq = (un) substituted C6-14 aryl, 5- to 14-membered heterocyclic group, C1-8 alkyl, C3-8 alicyclic hydrocarbyl, C6-14 aryl-C1-6 alkyl, 5- to 14-membered heteroaryl-C1-6 alkyl, (CH2)gSO2 (g = 1-8), (CH2) faCH: CH(CH2) fb (fa, fb = 0, 1,2,3), etc.; and Tg1 = a group of the general formula -Eg-CO-NRg1(Zg) or Q; wherein Eg = a single bond, (un) substituted NH; Rg1 = H, (un) substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 aliph. hydrocarbyl, etc.; Zg = C1-8 alkyl, C3-8 alicyclic hydrocarbyl, C6-14 aryl, etc.; Zg1, Zg2 = (a) a single bond, (b) C1-6 alkylene optionally having ≥1 atoms selected from O, S, and N in the middle or the terminus of the chain and optionally substituted with oxo, (c) (un)substituted C2-6 alkenyl] are prepd. These compds. are also inhibitors of vascular endothelial growth factor receptor kinase (VEGFR2 kinase) and are useful as antitumor agents against hemangioma, pancreatic cancer, stomach cancer, colon cancer, breast cancer, prostate cancer, lung cancer, brain tumor, leukemia, or ovarian cancer, as cancer metastasis inhibitors, and for the treatment of retina neovascularization, diabetic retinopathy, atherosclerosis, or inflammatory diseases such as osteoarthritis, rheumatoid arthritis, psoriasis, or delayed hypersensitivity. Thus, to soln. of 334 mg 4-[6-(4-benzyloxyphenyl)-7-(2trimethylsilylethoxymethyl) -7H-pyrrolo[2,3-d]pyrimidin-4-yloxy] -2chlorophenylamine in 4 mL DMF were added 0.066 mL pyridine and 0.102 mL Ph chlorocarbonate and stirred at room temp. for 2.5 h to give 330 mg N-[4-[6-(4-benzyloxyphenyl)-7-(2-trimethylsilylethoxymethyl)-7Hpyrrolo[2,3-d]pyrimidin-4-yloxy]-2-chlorophenyl]-N'-cyclopropylurea which (260 mg) was hydrogenolyzed over platinum oxide in ethanol overnight to give 160 mg N-[4-[6-(4-hydroxyphenyl)-7-(2-trimethylsilylethoxymethyl)-7Hpyrrolo[2,3-d]pyrimidin-4-yloxy]-2-chlorophenyl]-N'-cyclopropylurea (I). I showed IC50 of 0.02 nM for inhibiting the vascular endothelial growth factor (VEGF)-stimulated sandwich tube formation in vascular endothelial cell.

## IT 417713-01-0P 417713-68-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of urea derivs. contg. nitrogenous arom. ring compds. as
angiogenesis inhibitors for prevention or treatment of diseases)
RN 417713-01-0 HCAPLUS
CN Urea, N-[4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]-N'-1Himidazol-2-yl- (9CI) (CA INDEX NAME)

RN <u>417713-68-9</u> HCAPLUS

CN Urea, N-1H-benzimidazol-2-yl-N'-[4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

IT 4930-03-4, Phenylcarbamic acid phenyl ester

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of urea derivs. contg. nitrogenous arom. ring compds. as angiogenesis inhibitors for prevention or treatment of diseases)

RN 4930-03-4 HCAPLUS

CN Carbamic acid, phenyl-, phenyl ester (9CI) (CA INDEX NAME)

RN

CN

RN 65141-04-0 HCAPLUS

CN Carbamic acid, (4-fluorophenyl)-, phenyl ester (9CI) (CA INDEX NAME)

RN 347151-53-5 HCAPLUS

CN Carbamic acid, [4-[(6,7-dimethoxy-4-quinolinyl)oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417721-09-6 HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417721-10-9 HCAPLUS

CNCarbamic acid, [4-[[6-cyano-7-(2-methoxyethoxy)-4-quinolinyl]oxy]-2fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417721-11-0 HCAPLUS

Carbamic acid, [4-[(6-cyano-7-methoxy-4-quinolinyl)oxy]phenyl]-, phenyl CNester (9CI) (CA INDEX NAME)

RN 417721-13-2 HCAPLUS

CNCarbamic acid, [3-(methylsulfonyl)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

$$\mathsf{Me} = \bigcup_{0}^{0} \mathsf{NH} = \bigcup_{0}^{0} \mathsf{OPh}$$

RN 417721-32-5 HCAPLUS CN Carbamic acid, [4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417721-91-6 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-2-pyridinyl]amino]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 417722-40-8 HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-7-(2-methoxyethoxy)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} - \text{CH}_2 - \text{CH}_2 - \text{O} \\ \text{MeO} - \text{C} \\ \text{O} \\$$

RN 417722-53-3 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-3-methylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-83-9 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-87-3 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-(2-methoxyethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-91-9 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-(2-methoxyethoxy)-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN417722-95-3 HCAPLUS

Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-CNchlorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417722-99-7 HCAPLUS

Carbamic acid, [4-[[6-(aminocarbonyl)-7-(phenylmethoxy)-4-quinolinyl]oxy]-CN2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

417723-05-8 HCAPLUS RN

Carbamic acid, [4-[[6-(aminocarbonyl)-7-(phenylmethoxy)-4-quinolinyl]oxy]-CN2-chlorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417723-09-2</u> HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-chloro-4-[(phenoxycarbonyl)amino]phenoxy]-7-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 417723-58-1 HCAPLUS

CN Carbamic acid, [4-[[2-[(1-oxobutyl)amino]-4-pyridinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417723-70-7</u> HCAPLUS CN Carbamic acid, [4-[[

Carbamic acid, [4-[[7-methoxy-6-[(methylamino)carbonyl]-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417723-73-0</u> HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-methylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-76-3 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2-(trifluoromethyl)phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-78-5 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2,3-dimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417723-81-0 HCAPLUS

CN Carbamic acid, [4-[[6-(aminocarbonyl)-7-methoxy-4-quinolinyl]oxy]-2,5-dimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417724-07-3</u> HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-[(2R)-oxiranylmethoxy]-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 417724-17-5 HCAPLUS

CN Carbamic acid, [2-chloro-5-[[6-cyano-7-[(2R)-2-hydroxy-3-(1-pyrrolidinyl)propoxy]-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 417724-33-5 HCAPLUS

CN Carbamic acid, [4-[(6,7-dimethoxy-4-quinolinyl)oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417724-40-4</u> HCAPLUS

CN Carbamic acid, [4-[[6-cyano-7-[3-(1-piperidinyl)propoxy]-4-quinolinyl]oxy]-2-fluorophenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-41-5 HCAPLUS

CN Carbamic acid, [2-chloro-4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 417724-46-0 HCAPLUS

CN Carbamic acid, [2-chloro-4-[[6-[(methylamino)carbonyl]-7-(phenylmethoxy)-4-quinolinyl]oxy]phenyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN <u>417724-54-0</u> HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[6-cyano-4-[3-fluoro-4-[(phenoxycarbonyl)amino]phenoxy]-7-quinolinyl]oxy]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 417724-59-5 HCAPLUS

CN 6-Quinolinecarboxylic acid, 4-[3-fluoro-4-[(phenoxycarbonyl)amino]phenoxy]-7-methoxy-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ - \\ 0 \\ \text{PhO} \\ - \\ - \\ \text{N} \\ \text{N} \\ \\ \text{N} \\ \\ \text{PhO} \\ - \\ - \\ \text{NH} \\ \\ \end{array}$$

RN 417724-65-3 HCAPLUS

Carbamic acid, [4-[[6-cyano-7-(phenylmethoxy)-4-quinolinyl]oxy]-2,3-CNdimethylphenyl]-, phenyl ester (9CI) (CA INDEX NAME)

417724-88-0 HCAPLUS RN

1-Piperidinecarboxylic acid, 4-[2-[[4-[3-chloro-4-CN[(phenoxycarbonyl)amino]phenoxy]-2-pyridinyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

17

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN HCAPLUS L26 ANSWER 7 OF 21

References ACCESSION NUMBER:

2001:468189 HCAPLUS

DOCUMENT NUMBER: 135:61321

Methods for the solid phase synthesis of combinatorial TITLE:

libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivatives for use as

peptidomimetics

Laborde, Edgardo; Matsumoto, Yukiharu INVENTOR(S):

Telik, Inc., USA PATENT ASSIGNEE(S):

U.S., 18 pp. SOURCE:

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO	ο.	DATE
US_6251689	B1	20010626		US 1999-31356	В	19990514
US 2001024833	A1	20010927		US 2001-77564	4	20010205
PRIORITY APPLN. INFO.	:		US	1998-85465P	P	19980514
			US	1999-313568	A1	19990514

OTHER SOURCE(S): CASREACT 135:61321

The present invention provides an efficient and versatile method for the synthesis and screening of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles, and derivs. thereof. Thus, resin-bound 4-carboxybenzaldehyde in DMA is treated with 1,2-phenylenediamine and TCNE to give 2-(4-carboxyphenyl)benzimidazole. In order to expedite the synthesis of large arrays of compds. possessing these core structures, a general methodol. for solid phase synthesis of these derivs. is provided. Arrays of benzimidazoles, benzoxazoles, benzothiazoles, and derivs. thereof useful as peptidomimetics and for the identification of agents having antifungal, antiviral, antimicrobial, anticoagulant, and antiulcer activity, or use in the treatment of inflammation, hypertension, cancer, and other conditions can be prepd. by this method.

IT 345958-22-7D, resin bound

RL: RCT (Reactant); RACT (Reactant or reagent)
(methods for the solid phase synthesis of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivs. for use as peptidomimetics)

RN 345958-22-7 HCAPLUS

CN Benzoic acid, 3,4-bis[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 345958-14-7P 345958-15-8P 345958-17-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(methods for the solid phase synthesis of combinatorial libraries of benzimidazoles, benzoxazoles, benzothiazoles and derivs. for use as peptidomimetics)

RN <u>345958-14-7</u> HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[(phenylamino)carbonyl]amino](9CI) (CA INDEX NAME)

RN 345958-15-8 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[[[3-(trifluoromethyl)phenyl]amino] carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 345958-17-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[[(phenylamino)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 25 THERE AR

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2000:666713 HCAPLUS

DOCUMENT NUMBER:

133:252426

TITLE:

Preparation of aromatic heterocyclic ureas as

antiinflammatory agents

INVENTOR (S):

Betageri, Rajashehar; Breitfelder, Steffen; Cirillo, Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.; Kirrane, Thomas M.; Moriak, Monica H.; Moss, Neil; Patel, Usha R.; Proudfoot, John R.; Regan, John R.; Sharma, Rajiv; Sun, Sanxing; Swinamer, Alan D.;

Takahashi, Hidenori

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA

ADDITCATION NO

שתיעת

SOURCE:

PCT Int. Appl., 282 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

KIND DATE

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

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V	VO 2000055139				A	2	2000	0921		W	200	00-U	S386!	5	2000	0216		
V	NO 2	O 2000055139				.3 20010426												
		W:	ΑĖ,	AU,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	HR,	HU,	ID,	IL,	IN,	JP,	KR,
			KΖ,	LT,	LV,	MX,	NO,	NZ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	UZ,	VN,
			YU,	ZA														
		RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	ΝL,
			PT,	SE														
Ι	EP 1	P 1165516 A2 20020102								E	P 20	00-9	0729	5	2000	0216		
	R: AT. BE. CH. DE. DK					DK.	ES.	FR.	GB,	GR,	IT.	LI,	LU.	NL,	SE,	MC,	PT,	

GΙ

The title compds. (I) [wherein Ar1 = (un) substituted pyrrole, pyrrolidine, pyrazole, imidazole, oxazole, thiazole, furan, or thiophene; Ar2 = (un) substituted Ph, (tetrahydro) naphthyl, (tetrahydro) quinoline, (tetrahydro) isoquinoline, benzimidazole, benzofuran, indanyl, indenyl, or indole; W = O or S; X = (un) substituted cycloalkyl, cycloalkenyl, Ph, furan, thiophene, pyrrole, imidazolyl, pyridine, pyrimidine, (dihydro) pyridinone, (dihydro) maleimide, piperidine, piperazine, or pyrazine; Y = a bond or (un) substituted satd. or unsatd. alkyl optionally interrupted by O, NH, S(O), SO2, or S; Z = (un) substituted Ph, pyridine, pyrimidine, pyridazine, imidazole, (tetrahydro) furan, thiophene, (tetrahydro) pyran, 1,3-dioxolanone, 1,3-dioxanone, 1,4-dioxane, (thio) morpholine (sulfoxide), piperidine, cyclohexanone, pentamethylene sulfoxide, etc.] were prepd. for the treatment of diseases or pathol.

ΙI

conditions involving inflammation, such as chronic inflammatory diseases. Thus, coupling 2-cyclohexenone with 4-bromo-1-naphthylamine in the presence of Pd(PPh3)2Cl2, DPPP, and NaHCO3 in DMF, followed by conversion of the amine to an isocyanate using ClCOCl and immediate addn. of 1-(4-methylphenyl)-3-tert-butyl-1H-pyrazol-5-amine, gave the urea II. In a cytokine prodn. inhibition assay, preferred compds. of the invention showed IC50 < 10 .mu.M against TNF-.alpha. in lipopolysaccharide stimulated THF cells.

## IT 294851-78-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

RN 294851-78-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-(3-oxo-1-cyclohexen-1-yl)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 294848-43-4P 294848-46-7P 294848-49-0P 294848-51-4P 294848-53-6P 294848-55-8P 294848-58-1P 294848-61-6P 294848-64-9P 294848-67-2P 294848-70-7P 294848-73-0P 294848-76-3P 294848-79-6P 294848-82-1P 294848-85-4P 294848-88-7P 294848-91-2P 294848-94-5P 294848-96-7P 294848-98-9P 294849-00-6P 294849-02-8P 294849-04-0P 294849-06-2P 294849-08-4P 294849-10-8P 294849-12-0P 294849-14-2P 294849-16-4P 294849-18-6P 294849-20-0P 294849-22-2P 294849-24-4P 294849-26-6P 294849-28-8P 294849-30-2P 294849-32-4P 294849-34-6P 294849-36-8P 294849-38-0P 294849-40-4P 294849-42-6P 294849-44-8P 294849-46-0P 294849-48-2P 294849-50-6P 294849-52-8P 294849-54-0P 294849-56-2P 294849-58-4P 294849-60-8P 294849-62-0P 294849-64-2P 294849-66-4P 294849-68-6P 294851-79-9P 294851-81-3P 294851-83-5P 294851-85-7P 294853-11-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines) Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\sqcup$ RN

[4-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

CN

RN

CN

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Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$ [4-[2-(4-morpholinyl)ethyl]phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 294848-49-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\sqcup$  [3-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-51-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

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RN 294848-53-6 HCAPLUS

CN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[5-(4-morpholinylmethyl)-2-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-55-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[5-(4-morpholinylmethyl)-2-furanyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

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RN 294848-58-1 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA
INDEX NAME)

PAGE 2-A

RN 294848-61-6 HCAPLUS CN Urea, N-[3-(1,1-dime

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[6-(4- $\sqcup$ morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-64-9 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[3-[[2-(2-pyridinyl)ethyl]amino]-1-cyclohexen-1-yl]-1-naphthalenyl](9CI) (CA INDEX NAME)

RN 294848-67-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[ [4-[[(3-pyridinylmethyl)amino]methyl]phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-70-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[4-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

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RN 294848-73-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(4-hydroxybutyl)amino]-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-76-3 HCAPLUS

CN Benzamide, 5-[3-(1,1-dimethylethyl)-5-[[[[4-[6-(4-morpholinylmethyl)-3-[pyridinyl]-1-naphthalenyl]amino]carbonyl]amino]-1H-pyrazol-1-yl]-2-methyl-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294848-79-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[4-[(3-hydroxy-1-piperidinyl)methyl]phenyl]-1-naphthalenyl]- (9CI)

(CA INDEX NAME)□

PAGE 1-A

PAGE 2-A

Me N Bu-t

RN 294848-82-1 HCAPLUS

CN

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-□
N'-[4-[4-[(4-oxido-4-morpholinyl)methyl]phenyl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)□

PAGE 2-A

RN294848-85-4 HCAPLUS

CNUrea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-N'-[4-[3-(4-morpholinylmethyl)-1-cyclohexen-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-88-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-□ N'-[4-[3-hydroxy-4-[(tetrahydro-3-furanyl)methyl]phenyl]-1-naphthalenyl]-(9CI) (CA INDEX NAME)

PAGE 2-A

RN294848-91-2 HCAPLUS CN

Urea, N-[4-[ $\frac{1}{4}$ -[ $\frac{1}{4}$ -]-[ $\frac{1}{4}$ -[ $\frac{1}{4}$ -[ $\frac{1}{4}$ -]-[ $\frac{1}{4}$ -]-[ $\frac{1}{4}$ -[ $\frac{1}{4}$ -]-[ $\frac{1}$ (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} - \text{CH}_2 - \text{CH}_2 - \text{N} - \text{CH}_2 \\ \text{MeO} - \text{CH}_2 - \text{CH}_2 \end{array}$$

RN 294848-94-5 HCAPLUS

CN Urea, N-[4-[6-(3-cyanopropoxy)-3-pyridinyl]-1-naphthalenyl]-N'-[3-(1,1dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 294848-96-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[4-(4-morpholinylmethyl)-1-piperidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294848-98-9 HCAPLUS

CN Urea, N-[4-[4-[[bis(2-cyanoethyl)amino]methyl]phenyl]-1-naphthalenyl]-N'- $\square$  [3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)  $\square$ 

PAGE 1-A

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RN 294849-00-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[4-(2-furanylmethyl)-3-hydroxyphenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-02-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-N'-[4-[4-(4-thiomorpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-04-0 HCAPLUS

CN

3-Piperidinecarboxamide, 1-[[4-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-[pyridinyl)-1H-pyrazol-5-yl]amino]carbonyl]amino]-1-[naphthalenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-06-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-1 N'-[4-[4-[(2-methyl-3-oxo-1-piperazinyl)methyl]phenyl]-1-naphthalenyl]-(9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-08-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]-\(\text{N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-10-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[6-(4-hydroxybutoxy)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-12-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl) [1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-[6-(4- $\sqcup$  morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-14-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-16-4 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-[6- $\square$  (4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 294849-18-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[6-[(2,6-dimethyl-4-morpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl]-N(9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-20-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methoxy-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-22-2 HCAPLUS

CN Urea, N-[1-(6-amino-3-pyridinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 294849-24-4 HCAPLUS

CN Morpholine, 4-[[5-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-D pyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyridinyl]carbonyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-26-6 HCAPLUS

CN

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[6-(2-oxa-5-azabicyclo[2.2.1]hept-5-ylmethyl)-3-pyridinyl]-1- $\square$  naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-28-8 HCAPLUS

CN Urea, N-[4-[4-[((2-cyanoethyl)(3-pyridinylmethyl)amino]methyl]phenyl]-1naphthalenyl]-N'-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1Hpyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 294849-30-2 HCAPLUS

CN Urea, N-[4-[4-[(2-cyanoethyl) [(tetrahydro-2-furanyl)methyl]amino]methyl]pD henyl]-1-naphthalenyl]-N'-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-D 1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-32-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]-UN'-[4-[4-methoxy-6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]-(9CI) (CA INDEX NAME)

RN 294849-34-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]- $\square$  N'-[4-[6-[1-(4-morpholinyl)propyl]-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME) $\square$ 

PAGE 1-A

PAGE 2-A

RN 294849-36-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1'-methyl[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-Li
[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX
NAME)

PAGE 2-A

RN 294849-38-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-1-oxido-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl]- (9CI) (CA INDEX NAME)

RN 294849-40-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-42-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-pyrazol-5-yl]N'-[4-[5-[(tetrahydro-2H-thiopyran-4-yl)amino]pyrazinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-44-8 HCAPLUS

CN Acetamide, N-[5-[4-[[[[3-(1,1-dimethylethyl)-1-(6-methyl-3-pyridinyl)-1H-Description pyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyridinyl]- (9CI)

(CA INDEX NAME)

RN 294849-46-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1'-[3-(methylthio)propyl][1,4'-bi-1H-L]
pyrazol]-5-yl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]-

(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-48-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(1-oxido-4-thiomorpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

RN 294849-50-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-3-pyridinyl]-1-naphthalenyl](9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 294849-52-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-[2-(methylthio)-5-pyrimidinyl]-1H-pyrazol-5-y1]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 294849-54-0 HCAPLUS

Urea, N-[1-(2-amino-5-pyrimidinyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]- $\mathbb{N}$ '-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

294849-56-2 HCAPLUS RN

 $\label{eq:Urea} \textit{Urea, N-[3-(1,1-dimethylethyl)-1'-methyl[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-looper-left] } \\ = \textit{Urea, N-[3-(1,1-dimethyl)-1'-methyl[1,4'-bi-1H-pyrazol]-5-yl]-N'-[4-looper-left]-N$ CN[4-(4-morpholinylmethyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

294849-58-4 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$ CN[6-[(tetrahydro-1-oxido-2H-thiopyran-4-yl)amino]-3-pyridinyl]-1naphthalenyl] - (9CI) (CA INDEX NAME)

PAGE 2-A

294849-60-8 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$  [6-(4-thiomorpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA CNINDEX NAME)

294849-62-0 HCAPLUS RN

Morpholine, 4-[[5-[4-[[[[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-]]]]CNpyrazol-5-yl]amino]carbonyl]amino]-1-naphthalenyl]-2-pyrimidinyl]carbonyl]-(9CI) (CA INDEX NAME)

PAGE 1-A

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294849-64-2 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-fig]CN[2-(4-morpholinylmethyl)-5-pyrimidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

294849-66-4 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$  [6-[(1-oxido-4-thiomorpholinyl)methyl]-3-pyridinyl]-1-naphthalenyl]- (9CI) CN(CA INDEX NAME)

294849-68-6 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(2-methyl-5-pyrimidinyl)-1H-pyrazol-5-yl]- $\square$ CNN'-[4-[2-(4-morpholinylmethyl)-5-pyrimidinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

294851-79-9 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$ CN[3-(4-morpholinyl)-1-cyclohexen-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

294851-81-3 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\square$ CN[4-(4-morpholinyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

294851-83-5 HCAPLUS RN

Urea, N-[4-[4-[(dimethylamino)methyl]phenyl]-1-naphthalenyl]-N'-[3-(1,1- $\Box$ CNdimethylethyl) -1-(4-methylphenyl) -1H-pyrazol-5-yl] - (9CI) (CA INDEX NAME)

294851-85-7 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\sqcup$ CN[3-(4-morpholinyl)-1-cyclohepten-1-yl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

294853-11-5 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4- $\sqcup$  [3-(4-morpholinyl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME) CN

IT 261711-84-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

261711-84-6 HCAPLUS RN

Carbamic acid, [5-(1,1-dimethylethyl)-2-methylphenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

References

2000:493269 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 133:105343

Preparation of  $\beta$ -phenylalanine derivatives as TITLE:

integrin antagonists

Schoop, Andreas; Muller, Gerhard; Bruggemeier, Ulf; INVENTOR(S):

Schmidt, Delf; Stelte-Ludwig, Beatrix; Keldenich,

Jorg; Albers, Markus

Bayer A.-G., Germany PATENT ASSIGNEE(S): PCT Int. Appl., 129 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000041469	A2	20000720	WO 2000-EP120	20000111
WO 2000041469	<b>A3</b>	20001116		CI CI
W: AE, AL,	AM, AT	, AU, AZ, BA,	BB, BG, BR, BY, CA	, CH, CN, CR, CO,

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CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
              IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
               SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
               AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
               CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                      19990115
                          B1 20010918
                                                 US 1999-232738
     US 6291503
                                                  CA 2000-2360356 20000111
     CA 2360356
                                20000720
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                                                 EP 2000-903571
                                                                      20000111
                                20011024
     EP 1147079
                          A2
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO
                                                                      20000111
                                                  JP 2000-593094
                          T2
                                20021015
     JP 2002534439
                                                  US 2001-867835
                                                                      20010530
                          Α1
                                20011018
     US 2001031788
                          B2
                                20030708
     US 6589972
                                                                  A 19990115
                                              US 1999-232738
PRIORITY APPLN. INFO.:
                                                                  W 20000111
                                              WO 2000-EP120
                           MARPAT 133:105343
OTHER SOURCE(S):
GΙ
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 $\beta$ -Phenylalanine derivs. I [R1 = H, (un)substituted alkyl, cycloalkyl, AΒ aryl, heterocyclyl; R2, R3 = any group given for R1 or (un) substituted alkenyl or alkynyl, OH, alkoxy or R2 and R3 are bonded to each other; R4 = carboxy ester, SO2H, CHO, CONH2, C(S)NH2 or their derivs.; R5 = H, (un) substituted alkyl, cycloalkyl, aryl; R6 = any group given for R1 or is bonded to one of R7, R8 or R9; R7 is absent, H, (un) substituted alkyl or cycloalkyl, NO2, CN, CHO or CO2H or their derivs., or is bonded to one of R6, R8, or R9; R8, R9 = any group given for R1 or is bonded to one of R6, R7 or R9 or R8; R10, R11 = H, (un)substituted alkyl, cycloalkyl, or alkoxy, halo; L is a sulfonamide, amide, ether, ester, keto, urea, thioether, sulfoxide or sulfone unit optionally extended by one or two methylene groups; X is N, O or S] and their physiol. acceptable salts and stereoisomers were prepd. Thus, 3-[(phenylsulfonyl)amino]-3-[3-[(3guanidinophenyl)sulfonyl]phenyl]propionic acid trifluoroacetic acid salt, prepd. by a multistep procedure from 3-nitrobenzaldehyde, ammonium acetate, malonic acid, benzenesulfonyl chloride, 3-nitrobenzenesulfonyl chloride, and 1,3-bis(tert-butoxycarbonyl)-2-methyl-2-thiopseudourea, showed IC50 = 19 nM antagonist activity against integrin  $\alpha v \beta 3$ receptor.

IT 283613-04-7P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of  $\beta$ -phenylalanine derivs. as integrin antagonists)

RN 283613-04-7 HCAPLUS

Benzenepropanoic acid, 3-[[[3-[[(1H-benzimidazol-2-ylamino)carbonyl]amino]phenyl]sulfonyl]amino]-β[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

IT 283613-53-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of  $\beta$ -phenylalanine derivs. as integrin antagonists)

RN

Benzenepropanoic acid, 3-[[[3-[(ethoxythioxomethyl)amino]phenyl]sulfonyl]a mino]- $\beta$ -[(phenylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME) CN

ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

Citing References Text

2000:401817 HCAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

Heteroaryl-containing thiourea derivatives useful as

INVENTOR (S):

inhibitors of herpes viruses Bloom, Jonathan David; Digrandi, Martin Joseph;

Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

PCT Int. Appl., 164 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

WI THEORI	AIIC	,14 .														
PATENT N	Ο.		KIN	ID I	ATE				PPLIC							
WO 20000 W:	AE, CZ, IN, MD,	AL, DE, IS, MG, SL,	AM, DK, JP, MK, TJ,	AT, DM, KE, MN, TM,	AU, EE, KG, MW, TR,	ES, KP, MX, TT,	BA, FI, KR, NO, TZ,	BB, GB, KZ,	LC,	BR, GE, LK,	BY, GH, LR,	CA, GM, LS, RU,	CH, HR, LT, SD,	CN, HU, LU, SE, ZW,	LV, SG,	MA, SI,
RW: US 6166 US 6197	BY, GH, DK, CG,	KG, GM,	KZ, KE, FI, CM,	MD, LS, FR, GA,	RU, MW, GB, GN,	TJ, SD, GR,	SL, IE, ML,	SZ, IT, MR,	TZ, LU, NE.	UG, MC, SN,	ZW, NL, TD, 4478	AT, PT, TG	BE, SE, 1999	CH, BF, 1122 1122	CY, BJ,	DE,

HQ 6001013	В1	20010313	US 1999-444075 19991122
US 6201013	A1	20010313	10001006
EP 1140913	AT DE		FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
			FR, GB, GR, 11, D1, D0, M2, D2, 110, 11,
		FI, RO	TR 2001-20010159819991206
TR 200101598	T2	20011022	
	A	20011204	
JP 2002531558	T2	20020924	
AU 756043	B2	20030102	
US 6262082	B1	20010717	
US 6271236	Bl	20010807	US 2000-669943 20000926
ZA 2001004373	A	20020918	ZA 2001-4373 20010528
NO 2001002836	A	20010808	NO 2001-2836 20010608
BG 105580	A	20020131	BG 2001-105580 20010608
US 2003036653	A1	20030220	US 2002-99695 20020315
US 655561	B2	20030429	
PRIORITY APPLN. INFO	. :		US 1998-208540 A 19981209
			US 1998-150692P P 19981209
			US 1998-150698P P 19981209
			US 1998-155192P P 19981209
			US 1998-155240P P 19981209
			US 1998-208164 A 19981209
			US 1998-208561 A 19981209
			US 1999-444782 A3 19991122
			WO 1999-US28892 W 19991206
			US 2000-669535 A3 20000926
	347	DD3M 100.	20667

OTHER SOURCE(S):

MARPAT 133:30667

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 # H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; A = heteroaryl; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and

-7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 25 compds. in 2-4 bioassays. For instance, the pyridinylthiazolecarboxamide deriv. II had an IC50 of 0.001  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of heteroaryl-contg. thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT <u>71026-</u>66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heteroaryl-contg. thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of heteroaryl-contg. thiourea derivs. as

inhibitors of herpes viruses)

27339<u>0-64-0</u> HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME) CN

273390-92-4 HCAPLUS RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CNimidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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2

Full References Text

2000:401816 HCAPLUS ACCESSION NUMBER:

133:30666 DOCUMENT NUMBER:

Aryl- and heteroaryl-substituted thiourea derivatives TITLE:

useful as inhibitors of herpes viruses

Bloom, Jonathan David; Digrandi, Martin Joseph; INVENTOR(S):

Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

American Home Products Corporation, USA PATENT ASSIGNEE(S):

PCT Int. Appl., 159 pp. SOURCE:

CODEN: PIXXD2

Patent DOCUMENT TYPE:

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE							A1	PPLI	CATIO	ON NO	). I	DATE			
WO 2000034	268	A:	1 2	20000	0615							1999:			
W: AE	AT.	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
C7.	DE.	DK.	DM.	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	ıμ,
TN	, IS,	JP.	KE.	KG.	KP.	KR.	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,
MD	, MG,	MK.	MN.	MW.	MX.	NO.	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,
SK	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,
ВУ	, KG,	KZ,	MD,	RU,	ТJ,	TM									
RW: GH	. GM.	KE.	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,
DK	, ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG BR 1999-15993 20010904 A BR 9915993 EP 1999-965131 19991206 20011004 A1 EP 1137647 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 2000-586715 19991206 20020924 T2 JP 2002531557 20010525 ZA 2001-4318 Α 20020826 ZA 2001004318 20010608 NO 2001-2837 20010719 NO 2001002837 Α A 19981209 US 1998-207961 PRIORITY APPLN. INFO.: WO 1999-US28838 W 19991206

OTHER SOURCE(S):

MARPAT 133:30666

GΙ

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

Title compds. I and related compds. and their pharmaceutical salts are AB disclosed [wherein A = heteroaryl; R1-R4 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, cyano; R1R2 or R3R4 = C5-7 aryl fusion; G = aryl or heteroaryl; and X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph or PhCH2; n =1-6]. The compds. are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), and varicella-zoster virus (VZV), as well as (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 35 compds. in 2-4 bioassays. For instance, the pyridine deriv. II had an IC50 of 0.018  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture.

# IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CN ester (9CI) (CA INDEX NAME)

RN 273384-74-0 HCAPLUS

CN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heteroaryl thiourea derivs. as inhibitors

of herpes viruses)

RN 71026-66-9 HCAPLUS

CN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

RN 273390-64-0 HCAPLUS

CN Benzamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

RN 273390-92-4 HCAPLUS

CN 1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} S \\ NH - C - NH \end{array}$$

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

1

# References

ACCESSION NUMBER:

DOCUMENT NUMBER:

INVENTOR(S):

TITLE:

2000:401809 HCAPLUS

133:30657

Heterocyclic carboxamide-containing thiourea

derivatives containing a substituted phenylenediamine

group, useful as inhibitors of herpes viruses

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas

Richard; Lang, Stanley Albert; Ross, Adma Antonia;

Terefenko, Eugene Anthony; O'Hara, Bryan Mark

American Home Products Corporation, USA

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

NI INI ORILI	1 1 0 1												
PATENT NO		KIND	DATE		AI	PLIC	CATIO	N NC	). I	OATE			
_	4261 E, AL,	A3 AM, AT	200201 AU, AU, A	131 AZ, BA, ES FI.	BB,	GD,	BR, GE,	BY,	CA, GM,	CH,	CN, HU,	,	
I: M: S	N, IS, D, MG, K, SL,	JP, KE MK, MN TJ, TN	E, KG, 1 N, MW, 1 M, TR, '	KP, KR, MX, NO, TT, TZ,	KZ,	LC,	LK, PT.	LК, RO,	RU,	SD,	SE,	SG,	SI,
RW: G D	H, GM, K, ES,	KE, LS FI, FI	R, GB, A. GN,	SD, SL, GR, IE, GW, ML,	MR,	NE,	SN,	TD,	TG	BE, SE,	21,	CY, BJ,	DE, CF,
US 616602 US 619780 US 620101 EP 114439 EP 114439	.3 .9	B1 B1 A2	20010 20010 20011	0306 0313 L017	U E	S 19 S 19 P 19	99-4 99-4 99-9	4407 6721	<u>5</u> 3	1999 1999 1999	1122 1122 1206		PT,

IE, SI, LT	r, LV,	FΙ,	RO				
BR 9916043	A	2001	1204		BR 1999-16043		19991206
JP 2002533301	T2	20023	1008		JP 2000-586708	3	19991206
US 6262082	В1	2001	0717		US 2000-669483	3	20000925
US 6271236	В1	2001	0807		US 2000-66994:	3	20000926
ZA 2001004322	A	2002	1025		ZA 2001-4322		20010525
NO 2001002835	A	2001	0719		NO 2001-2835		20010608
US 2003036653	A1	2003	0220		US 2002-99695		20020315
US 6555561	B2	2003					
PRIORITY APPLN. INFO.:	22			US	1998-208164	A	19981209
PRIORITI APPEN. INTO				US	1998-150692P	Р	19981209
				US	1998-150698P	P	19981209
				US	1998-155192P	P	19981209
				US	1998-155240P	P	19981209
				US	1998-208540	Α	19981209
				US	1998-208561	Α	19981209
				US	1999-444782	A3	19991122
				WO	1999-US28916	W	19991206
				US	2000-669535	А3	20000926

OTHER SOURCE(S):

MARPAT 133:30657

$$R^4$$
 $R^5$ 
 $R^9$ 
 $R^{10}$ 
 $R$ 

$$\begin{array}{c|c} \text{MeO} & \text{C1} & \text{C1} \\ \\ \text{MeO} & \text{HN} & \\ \text{S} & \text{O} & \text{O} & \text{II} \end{array}$$

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AΒ alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero) aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion, provided that at least 1 of R9-R12  $\neq$  H; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std.

methods are listed, with biol. data for 18 compds. in 4 bioassays. For instance, the N-(4-thioureidophenyl)furan-2-carboxamide deriv. II had an IC50 of 0.4  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture, and 0.5  $\mu g/mL$  against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of heterocyclic carboxamide-contg. and phenylenediamine contg. thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CN ester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heterocyclic carboxamide-contg. and phenylenediamine-contg. thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of heterocyclic carboxamide-contg. and

phenylenediamine-contg. thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

273390-92-4 HCAPLUS RN

CN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1Himidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

#### HCAPLUS COPYRIGHT 2004 ACS on STN ANSWER 13 OF 21 L26

Citing Full References Text

ACCESSION NUMBER:

2000:401808 HCAPLUS

DOCUMENT NUMBER:

133:30588

TITLE:

Alpha-methylbenzyl-containing thiourea derivatives

containing a phenylenediamine group, useful as

inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia;

O'Hara, Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

PCT Int. Appl., 168 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	DATE		_			ON NO		OATE  1999:	1206			
WO 2000034260	112	20000615		M	J 15.	99-01	J <u>Z</u> 00.					
WO 2000034260		20000908						<b>G</b> 3	CIT	CN	CD.	CII
W: AE, AL,	AM, AT,	AU, AZ,	BA,	BB,	ВG,	BR,	BY,	CA,	CH,	CN,	CR,	CO,
CZ. DE.	DK, DM,	EE, ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	Hυ,	ID,	ıш,
TN TS.	JP. KE.	KG, KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	ъU,	LV,	MΑ,
MD. MG.	MK. MN.	MW, MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,
SK, SL,	TJ, TM,	TR, TT,	TZ,	UA,	ŪĠ,	UΖ,	VN,	YU,	ZA,	ZW,	AM,	AZ,

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BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                          19991206
                                                    BR 1999-16084
                                  20010904
     BR 9916084
                           А
                                                                          19991206
                                                     EP 1999-963022
                                  20011004
                            A2
     EP 1137645
                           Вl
                                  20040526
     EP 1137645
               AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO
                                                                          19991206
                                                     JP 2000-586707
                            T2
                                  20020924
     JP 2002531555
                                                                          20010528
                                                     ZA 2001-4376
                                  20020828
      ZA 2001004376
                            Α
                                                                          20010608
                                                     NO 2001-2833
                                  20010802
     NO 2001002833
                            Α
                                                                      A 19981209
                                                 US 1998-208902
PRIORITY APPLN. INFO.:
                                                 WO 1999-US28839 W
                                                                         19991206
```

OTHER SOURCE(S):

MARPAT 133:30588

GT

$$\operatorname{Br} \longrightarrow \operatorname{HN} \longrightarrow \operatorname{NH} \longrightarrow \operatorname{NH}$$

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AB alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero) aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5  $\neq$  H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or fused bicyclic aryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 320 compds. in 1-4 bioassays. For instance, the [[(phenylethyl)thioureido]phenyl]benzofurancarboxamide deriv. II had an IC50 of 1.3  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture, and 0.10  $\mu g/mL$  against VZV in an ELISA assay.

IT 273384-69-3P 273384-74-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent) (intermediate; prepn. of  $\alpha$ -methylbenzyl-contg. thiourea derivs. as inhibitors of herpes viruses) 273384-69-3 HCAPLUS RN Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CN(CA INDEX NAME) ester (9CI)

273384-74-0 HCAPLUS RN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of  $\alpha\text{-methylbenzyl-contg.}$  thiourea derivs. as inhibitors of herpes viruses) 71026-66-9 HCAPLUS RN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CNNAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of  $\alpha\text{-methylbenzyl-contg.}$  thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CNyl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

273390-92-4 HCAPLUS RN1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CN

imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

### Citing Text References

ACCESSION NUMBER: DOCUMENT NUMBER:

2000:401806 HCAPLUS 133:30733

TITLE:

CN

Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group,

useful as inhibitors of herpes viruses

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas Richard; Lang, Stanley Albert; Ross, Adma Antonia;

Terefenko, Eugene Anthony; O'Hara, Bryan Mark

American Home Products Corporation, USA

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 188 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

INVENTOR (S):

Patent English

TANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO. DATE
WO 2000034258	A2 20000615 A3 20011129 , AM, AT, AU, AZ,	BA BB. BG. BR. BY, CA, CH, CN, CR, CU,
CZ, DE IN, IS MD, MG SK, SI	, DK, DM, EE, ES, , JP, KE, KG, KP, , MK, MN, MW, MX, , TJ, TM, TR, TT,	KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
BY, KG RW: GH, GM	, KZ, MD, RU, TJ, , KE, LS, MW, SD, , FI, FR, GB, GR, CM, GA, GN, GW,	SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, ML, MR, NE, SN, TD, TG
	A2 20011017	EP 1999-963023 19991206
R: AT, B	CH, DE, DK, ES, LT, LV, FI, RO	FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

TR 200101664	Т2	20020321	TR 2001-200101664	119991206
JP 2002531554	T2	20020924	JP 2000-586705	19991206
ZA 2001004377	A	20021220	ZA 2001-4377	20010528
	A	20010807	NO 2001-2832	20010608
NO 2001002832 BG 105581	A	20011231	BG 2001-105581	20010608
PRIORITY APPIN. INFO.:	21	200225	US 1998-208559 A	19981209
PRIORILI APPEN. INIO			WO 1999-US28842 W	19991206

OTHER SOURCE(S):

MARPAT 133:30733

$$R^4$$
 $R^5$ 
 $X$ 
 $HN$ 
 $G$ 
 $NH$ 
 $G$ 

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AΒ alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5  $\neq$  H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph;  $G = R^2 + R^2 +$ monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 350 compds. in 1-4 bioassays. For instance, the thioureidophenylthiadiazolecarboxamide deriv. II had an IC50 of 0.0011  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RN

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CN ester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

CN

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) CN

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of heterocyclic carboxamide-contg. thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

Benzamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c} \mathsf{t}^{-\mathsf{B}\mathsf{u}} \\ \mathsf{N} \\ \mathsf{N}$$

273390-92-4 HCAPLUS RN

CN

 $\frac{1}{2}$ ,  $\frac{1}{3}$ -Thiadiazole-4-carboxamide, N-[4-[[[1-(1,1-dimethylethyl)-1Himidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

## Full References

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

2000:401786 HCAPLUS

133:30587

Benzamide-containing aryl thiourea derivatives useful

as inhibitors of herpes viruses

INVENTOR(S):

Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia;

O'Hara, Bryan Mark

PATENT ASSIGNEE(S):

SOURCE:

American Home Products Corporation, USA

PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	ENT 1	10.		KI	1D 1	DATE			AI	PPLIC	CATIO	ON NO	). 	DATE			
WO	20000	3423	38	Α:	1 :	20000	0615		M	199	99-US	32883	37	1999	1206	<b>~</b> -	GI I
	W:	ΛE	<b>Δ</b> Τ.	ΔM	ΔТ.	AII.	AZ.	BA.	BB,	ВG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
		C7	חדי	DΚ	DΜ	EE.	ES.	FI,	GB,	GD,	GE,	GH,	GM,	HK,	Hυ,	ΙD,	TL,
		TM	TS	JP.	KE.	KG.	KP,	KR,	KZ,	LC,	LК,	LR,	LS,	LΤ,	ъU,	ъ∨,	MIA,
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		SK	SI.	TJ.	TM.	TR.	TT,	TZ,	UA,	UG,	UΖ,	VN,	YU,	ZA,	ZW,	AM,	AZ,
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	D M.	CH	CM	KE	LS.	MW.	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,
	KW.	DK	EC.	ET.	FR	GB.	GR.	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CC,	CT,	CM	GD.	GN,	GW.	ML.	MR,	NE,	SN,	TD,	TG				
110	6166		C + ,	7	GH,	2000	1226	,	Ü	s 19	99-4	4478	2	1999	1122		
US	6197	028		n D	1	2001	0306		Ū	S 19	99-4	4700	6	1999	1122		
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	6207					2001								1999	1122		
	6255			В	_					S 19				1999			
	6262			В	_	2001			_	S 19							
	6335			В	1	2002	0101										
BR	9916	086			-	2001	0904		<u> </u>	K 19	99-1	6000		1999 1999	1206		
EP	1137	632		A	.1	2001	1004		<u>E</u>	P 19	99-9	6302					рт
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	, 11	ьU,	NL,	ъĿ,	IIIC,	F 1 ,

IE, SI, L	T, L	V, FI, RO			
TR 200101597	T2	20011022	TR 2001-200101	L597	19991206
JP 2002531545	T2	20020924	JP 2000-586686	5	19991206
NZ 512108	A	20030926	NZ 1999-512108	3	19991206
US 6262082	В1	20010717	US 2000-669483	3	20000925
US 6271236	В1	20010807	US 2000-669943	3	20000926
US 6403617	В1	20020611	US 2000-66953	5	20000926
US 6407123	В1	20020618	US 2000-67018	2	20000926
US 6426355	В1	20020730	US 2000-67148	5	20000927
US 6407249	В1	20020618	US 2000-68401	1_	20001229
US 6410571	B1	20020625	US 2000-68477	3	20001229
US 2002026055	A1	20020228	US 2001-80451	0	20010312
US 6380243	В2	20020430			
US 2001039348	A1	20011108	US 2001-84542	8	20010430
US 6462055	В2	20021008			
ZA 2001004144	A	20020821	ZA 2001-4144		20010521
NO 2001002838	A	20010808	NO 2001-2838		20010608
BG 105583	A	20011231	BG 2001-10558	3	20010608
US 2003036653	A1	20030220	US 2002-99695		20020315
US 6555561	В2	20030429			
PRIORITY APPLN. INFO.			US 1998-208561	Α	19981209
			US 1998-228805P	Р	19981209
			US 1998-228808P	P	19981209
			US 1998-228809P	P	19981209
			US 1998-150692P	Ρ	19981209
			US 1998-150698P	P	19981209
			US 1998-155192P	P	19981209
			US 1998-155240P	P	19981209
			US 1998-208164	Α	19981209
			US 1998-208540	Α	19981209
			US 1999-444734	Α3	19991122
			US 1999-444782	А3	19991122
			US 1999-444896	Α3	19991122
			US 1999-447006	Α3	19991122
			WO 1999-US28837	W	19991206
			US 2000-669535	А3	20000926

OTHER SOURCE(S):

MARPAT 133:30587

$$\begin{array}{c} \text{MeO} \\ \\ \text{MeO} \\ \\ \text{HN} \\ \\ \text{S} \\ \\ \text{O} \\ \\ \text{II} \\ \end{array}$$

AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8,

NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl fusion, provided that at least 1 of R9-R12  $\neq$  H; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or fused bicyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 75 compds. in 2-4 bioassays. For instance, the thioureidophenylbenzamide deriv. II had an IC50 of 1.5  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture, and 0.04 µg/mL against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

273384-69-3 HCAPLUS RÑ

Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl CNester (9CI) (CA INDEX NAME)

273384-74-0 HCAPLUS RN

Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, CN1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

71026-66-9 HCAPLUS RN

Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX CN

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of benzamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

CN

Benzamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

273390-92-4 HCAPLUS RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CNimidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-imidazol-2-CN yl]amino]thioxomethyl]amino]phenyl] - (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

Citing Full References Text ACCESSION NUMBER:

2000:401785 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes

INVENTOR(S):

Bloom, Jonathan David; Digrandi, Martin Joseph;

Dushin, Russell George; Lang, Stanley Albert; O'Hara,

Bryan Mark

PATENT ASSIGNEE(S):

American Home Products Corporation, USA

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ \_ \_ \_ \_ \_\_\_\_\_ \_\_\_\_\_\_ WO 1999-US28844 19991206 WO 2000034237 20000615 A2 WO 2000034237 20001123 **A3** W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG A2 20011004 EP 1999-965132 19991206 EP 1137633 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO BR 1999-16041 19991206 A 20011204 BR 9916041 JP 2000-586685 19991206 T2 20020924 JP 2002531544 ZA 2001-4142 20010521 20021025 Α ZA 2001004142 NO 2001-2834 20010608 20010807 NO 2001002834 Α US 1998-208316 A 19981209 PRIORITY APPLN. INFO.: WO 1999-US28844 W 19991206 MARPAT 133:30586

OTHER SOURCE(S):

GI

$$R^4$$
 $R^5$ 
 $R^9$ 
 $R^{10}$ 
 $R$ 

Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 AB alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero) aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5  $\neq$  H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; R9-R12 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R9R10 or R11R12 = C5-7 aryl

fusion; W = 0, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = C1-6 alkyl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases assocd. with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepd. by std. methods are listed, with biol. data for approx. 160 compds. in 4 bioassays. For instance, the thioureidophenylacetamide deriv. II had an IC50 of 0.8  $\mu g/mL$  against HCMV wild-type in human foreskin fibroblast cell culture, and 2  $\mu g/mL$  against HSV in an ELISA assay.

IT 273384-69-3P 273384-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of acetamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

RN 273384-69-3 HCAPLUS

CN Carbamic acid, [4-[(2-fluorobenzoyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273384-74-0 HCAPLUS

CN Carbamic acid, [4-[[2-(methylsulfinyl)benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$NH = C = 0Bu - t$$

$$C = NH$$

IT 71026-66-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (starting material; prepn. of acetamide-contg. aryl thiourea derivs. as
 inhibitors of herpes viruses)

RN 71026-66-9 HCAPLUS

CN Carbamic acid, (4-aminophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 273390-64-0P 273390-92-4P 273390-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compd.; prepn. of acetamide-contg. aryl thiourea derivs. as inhibitors of herpes viruses)

273390-64-0 HCAPLUS RN

CN

Benzamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2yl]amino]thioxomethyl]amino]phenyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{t-Bu} \\ \text{N} \\ \text{NH} - \text{C-NH} \\ \end{array} \begin{array}{c} \text{NH} - \text{C} \\ \text{F} \\ \end{array}$$

273390-92-4 HCAPLUS RN

1,2,3-Thiadiazole-4-carboxamide, N-[4-[[[[1-(1,1-dimethylethyl)-1H-CN imidazol-2-yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

273390-93-5 HCAPLUS RN

2-Furancarboxamide, N-[4-[[[1-(1,1-dimethylethyl)-1H-imidazol-2-]]]CN yl]amino]thioxomethyl]amino]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN L26

Citing Full References Text

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

2000:335391 HCAPLUS

132:347569

Preparation gastrin and cholecystokinin receptor

ligands

INVENTOR(S):

Kalindjian, Sarkis Barret; Buck, Ildiko Maria; Linney, Ian Duncan; Wright, Paul Trevor; McDonald, Iain Mair; Steel, Katherine Isobel Mary; Hull, Robert Antony David; Roberts, Sonia Patricia; Gaffen, John David; Vinter, Jeremy Gilbert; Walker, Martin Keith; Black, James Whyte; Watt, Gillian Fairfull; Harper, Elaine Anne; Shankley, Nigel Paul; Tozer, Matthew John; Dunstone, David John; Pether, Michael John; Lilley, Elliot James; Sykes, David Andrew; Low, Caroline Minli Rachel; Griffin, Eric Peter; Wright, Laurence

James Black Foundation Limited, UK PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 210 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

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APPLICATION NO. DATE
                     KIND DATE
    PATENT NO.
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                                           -----
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                    A1 20000518
    WO 2000027823
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            SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
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        RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
            DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                                          EP 1999-954196
                                                             19991109
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                      A1
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                       Α
                                           NO 2001-2288
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    NO 2001002288
                                          US 2001-831385 20010802
                            20021112
     US 6479531
                       В1
                                        GB 1998-24536 A 19981109
PRIORITY APPLN. INFO.:
                                        GB 1999-16786 A 19990716
                                        WO 1999-GB3733 W 19991109
OTHER SOURCE(S): MARPAT 132:347569
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Title compds. (I) [wherein X and Y = independently N, N(R5), CH, S, or O; n = 1-4; Z = (NR7)aCO(NR8)b, CONR7CH2CONR8, CO2, CH2CH2, CH=CH, CH2N(R8), or a bond; a and b = independently 0 or 1; Q = R9V (un) substitutedphenyl(alkyl); V = CONHSO2Ph, SO2NHCOPh, CH2OH, etc.; R1 = H or (halo) hydrocarbyl where  $\leq$  3 C atoms may be replaced by N, O, and/or S atoms; R2 = H, Me, Et, Pr, or OH; R3 = H, Me, Et, or Pr; or 2 adjacent R3 groups form a carbocyclic ring when n > 1; or R2 and R3 on the same C atom together = :0 ; R4 = (halo)hydrocarbyl where  $\leq$  2 C atoms may be replaced by N, O, and/or S atoms; R5 = H, Me, Et, Pr, benzyl, OH, or carboxymethyl (esters); R7 and R8 = independently H, Me, Et, Pr, or benzyl; R9 = CH2, CH2CH2, or (un) substituted phenylmethylene; or R8 and R9, together with the adjacent N, form a substituted piperidine or pyrrolidine] and their pharmaceutically acceptable salts were prepd. Examples include syntheses and biol. data for 314 compds. Thus, 2-adamantan-1-ylmethyl-5-phenyl-1H-pyrrole-3-carboxylic acid (3-step prepn. given) was coupled with 5-aminoisophthalic acid dibenzyl ester (45%), followed by deprotection (98%) to give II. II had pKi of 6.72 for binding at the CCKB mouse cortical membranes and pKb of 6.33 for gastrin antagonist activity.

IT 269071-04-7P 269071-45-6P

RN 269071-45-6 HCAPLUS
CN Benzoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-[[[2-(2-

methylphenyl) -5-(2-tricyclo[3.3.1.13,7]dec-1-ylethyl) -1H-imidazol-4-yl]carbonyl]amino] - (9CI) (CA INDEX NAME)

IT <u>269072-17-5</u>

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. gastrin and cholecystokinin receptor ligands)

RN 269072-17-5 HCAPLUS

CN Benzoic acid, 5-amino-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CN

IT 269068-26-0P 269073-03-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. gastrin and cholecystokinin receptor ligands)

269068-26-0 HCAPLUS RN

Benzoic acid, 3-[[[[2-(2-methylphenyl)-5-(2-tricyclo[3.3.1.13,7]dec-1ylethyl)-1H-imidazol-4-yl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)

RN

269073-03-2 HCAPLUS D-Glucitol, 1-deoxy-1-(methylamino)-, 3-[[[[2-(2-methylphenyl)-5-(2tricyclo[3.3.1.13,7]dec-1-ylethyl)-1H-imidazol-4yl]amino]carbonyl]amino]benzoate (salt) (9CI) (CA INDEX NAME)

1 CM

269068-26-0 CRN C30 H34 N4 O3 CMF

CRN 6284-40-8 CMF C7 H17 N O5

Absolute stereochemistry.

MeNH S R R R OH

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

1999:425745 HCAPLUS

DOCUMENT NUMBER:

131:87909

TITLE:

Inhibition of p38 kinase activity using substituted

heterocyclic ureas

INVENTOR (S):

Dumas, Jacques; Khire, Uday; Lowinger, Timothy Bruno; Paulsen, Holger; Riedl, Bernd; Scott, William J.; Smith, Roger A.; Wood, Jill E.; Hatoum-Mokdad, Holia;

Johnson, Jeffrey; Lee, Wendy; Redman, Aniko

Bayer Corporation, USA

PATENT ASSIGNEE(S):

PCT Int. Appl., 126 pp. CODEN: PIXXD2

SOURCE:

GΙ

Patent

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ \_ \_ \_ \_ \_\_\_\_\_ WO 1998-US26080 19981222 WO 9932111 A1 19990701 AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG CA 1998-2315720 19981222 19990701 CA 2315720 AΑ AU 1999-19971 19981222 19990712 AU 9919971 Α1 AU 739642 20011018 B2 EP 1998-964709 19981222 20001011 EP 1041982 A1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO JP 2000-525102 19981222 20011218 JP 2001526223 T2US 1997-995750 A 19971222 PRIORITY APPLN. INFO.: WO 1998-US26080 W 19981222 MARPAT 131:87909 OTHER SOURCE(S):

A method for treatment of p38-mediated disease other than cancer comprises AΒ administration of ANHCONHB [I; A = substituted isoxazolyl, pyrazolyl, thienyl, furyl; B = (substituted) mono-, di-, or tricyclic aryl, heteroaryl contg.  $\geq 1$  5-6 membered arom. structure contg. 0-4 N, O, or S atoms]. Reaction of 4-(4-pyridinylthio)aniline with 3-tert-butyl-5-isoxazolyl isocyanate in toluene gave title compd. II. an in vitro p38 kinase assay, I displayed IC50 values of 1-10  $\mu \text{M}.$ 

IT 135680-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of substituted heterocyclic ureas for treatment of p38 kinase-mediated diseases other than cancer) 135680-03-4 HCAPLUS

RNCarbamic acid, [4-[(4-aminophenyl)methyl]phenyl]-, 1,1-dimethylethyl ester CN(CA INDEX NAME)

IT 229002-05-5P 229003-23-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of substituted heterocyclic ureas for treatment of p38

kinase-mediated diseases other than cancer)

229002-05-5 HCAPLUS

RN

CN

Urea, N-[4-[(4-aminophenyl)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-[3-(1,1-dimethylethyl)]methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

229003-23-0 HCAPLUS RN

1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-CN 3-(1,1-dimethylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

$$t-Bu$$
 $N$ 
 $N$ 
 $CH_2$ 
 $0-C-NH$ 
 $C1$ 
 $C1$ 
 $C1$ 
 $C1$ 

RN 227623-23-6 HCAPLUS
CN Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[(3-hydroxyphenyl)methyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229001-93-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 229001-95-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-pyridinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN <u>229001-97-2</u> HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

RN 229001-98-3 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229002-00-0 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-CN (phenylthio)phenyl] - (9CI) (CA INDEX NAME)

t.-Ru RN

229002-01-1 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-CNhydroxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN

229002-02-2 HCAPLUS

Urea, N-[4-[(4-butoxyphenyl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-CN methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu RN

229002-03-3 HCAPLUS

Butanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

t-Bu RN

229002-04-4 HCAPLUS

Carbamic acid, [4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CN yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME) (9CI)

t-Bu 229002-0

229002-06-6 HCAPLUS

CN Acetamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

229002-07-7 HCAPLUS

CN Butanoic acid, 4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

RN

229002-08-8 HCAPLUS

CN Propanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu´

RN 229002-09-9 HCAPLUS

CN Urea, N-[4-(4-aminophenoxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu RN

229002-10-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-

pyridinyloxy)phenyl] - (9CI) (CA INDEX NAME)

RN 229002-11-3 HCAPLUS

CN Carbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

t-Bu RN 229002-12-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-13-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-14-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 229002-15-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 229002-16-8 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-methylphenoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 229002-17-9 HCAPLUS

CN Urea, N-[3-(2-benzothiazolyloxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-18-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-phenyl-2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-19-1 HCAPLUS

CN Urea, N-[4-(2-benzothiazolylthio)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-20-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-(1,1-dimethylethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-21-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-[(trifluoromethyl)thio]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN

229002-22-6 HCAPLUS

CN Urea, N-[1,1'-biphenyl]-3-yl-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-24-8 HCAPLUS

CN Butanamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 229002-25-9 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-propoxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-26-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-27-1 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu RN

229002-28-2 HCAPLUS

CN 1H-Pyrazole-1-carboxylic acid, 3-(1,1-dimethylethyl)-5-[[[[4-[3-[(methylamino)carbonyl]phenoxy]phenyl]amino]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-Bu

229002-87-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[[(9H-fluoren-2-ylamino)carbonyl]amino]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 229002-97-5 HCAPLUS  $\label{eq:Urea} \mbox{Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2-hydroxyethyl)-1-(2-hydr$ CNlH-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu 229002-98-6 HCAPLUS RN

1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-CN3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

229002-99-7 HCAPLUS RN

1H-Pyrazole-1-acetamide, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-CN (1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)

229155-38-8 HCAPLUS RN

Urea, N-[4-[(4,5-dihydro-4-phenyl-5-thioxo-1,3,4-thiadiazol-2-CNyl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

229155-39-9 HCAPLUS RN

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4,5-CNdiphenyl-2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

229155-40-2 HCAPLUS RN

Urea, N-[4-([1,1'-biphenyl]-4-yloxy)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-CNdimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu

229155-41-3 HCAPLUS

RNUrea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-CN(phenylmethoxy)phenoxy]phenyl] - (9CI) (CA INDEX NAME)

t-Bu

229155-42-4 HCAPLUS

RNUrea, N,N''-(methylenedi-4,1-phenylene)bis[N'-[3-(1,1-dimethylethyl)-1-CN methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array} \begin{array}{c} \text{CH 2} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array} \begin{array}{c} \text{Me} \\ \text{N} \\ \text{Bu-t} \\ \end{array}$$

229155-43-5 HCAPLUS RN

Urea, N,N''-(oxydi-4,1-phenylene)bis[N'-[3-(1,1-dimethylethyl)-1-methyl-1H-CN pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229155-44-6 HCAPLUS

Propanamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu RN

229155-45-7 HCAPLUS

Acetamide, N-[4-[4-[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-]]]CN yl]amino]carbonyl]amino]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229155-46-8 HCAPLUS

Carbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CN yl]amino]carbonyl]amino]phenoxy]phenyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229155-47-9 HCAPLUS

Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-CN5-y1]- (9CI) (CA INDEX NAME)

t-Bu RN

229155-48-0 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-CN(trifluoromethyl)phenyl] - (9CI) (CA INDEX NAME)

t-Bu

229155-49-1 HCAPLUS RN

Urea, N-(3,5-dibromophenyl)-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-CN5-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & \\ & & \\ N \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\$$

RN 229155-50-4 HCAPLUS

CN Benzoic acid, 4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]-, butyl ester (9CI) (CA INDEX NAME)

t-Bu<sup>'</sup> RN 229155-5

229155-51-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylthio)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229155-52-6 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-pyridazinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu´

RN 229155-53-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 229155-54-8 HCAPLUS

CN Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229155-55-9 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(2,3-dichlorophenyl)- (9CI) (CA INDEX NAME)

RN 229155-56-0 HCAPLUS

CN Urea, N-[1-cyclohexyl-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 229155-69-5 HCAPLUS

CN Benzamide, 4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]-N-ethyl- (9CI) (CA INDEX NAME)

RN 229155-70-8 HCAPLUS

CN Benzamide, 4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]thio]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 229155-71-9 HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[[3-[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenyl]thio]- (9CI) (CA INDEX NAME)

RN 229155-81-1 HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-5-[4-[[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenoxy]- (9CI) (CA INDEX NAME)

IT 229003-22-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of substituted heterocyclic ureas for treatment of
p38 kinase-mediated diseases other than cancer)

RN 229003-22-9 HCAPLUS

CN Carbamic acid, (2,3-dichlorophenyl)-, 2-[5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-1H-pyrazol-1-yl]ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

1

## L26 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

INVENTOR(S):

1999:425740 HCAPLUS

131:73648

Inhibition of raf kinase using substituted

heterocyclic ureas

Dumas, Jacques; Khire, Uday; Lowinger, Timothy Bruno; Paulsen, Holger; Riedl, Bernd; Scott, William J.;

Smith, Roger A.; Wood, Jill E.; Hatoum-Mokdad, Holia;

Johnson, Jeffrey; Lee, Wendy; Redman, Aniko

PATENT ASSIGNEE(S):

SOURCE:

GΙ

Bayer Corporation, USA PCT Int. Appl., 163 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

Engi.

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	KIND DATE	APPLICATION NO.	DATE
		WO 1998-US26078	19981222
W: AL, AM,	AT, AU, AZ, BA, F	BB, BG, BR, BY, CA, CH,	CN, CU, CZ, DE,
DK, EE,	ES, FI, GB, GD, C	E, GH, GM, HR, HU, ID,	IL, IN, IS, JP,
KE, KG,	KP, KR, KZ, LC, I	LK, LR, LS, LT, LU, LV,	MD, MG, MK, MN,
MW, MX,	NO, NZ, PL, PT, F	RO, RU, SD, SE, SG, SI,	, SK, SL, TJ, TM,
		YU, ZW, AM, AZ, BY, KG,	
RW: GH, GM,	KE, LS, MW, SD, S	SZ, UG, ZW, AT, BE, CH	, CY, DE, DK, ES,
FI, FR,	GB, GR, IE, IT, I	LU, MC, NL, PT, SE, BF	, BJ, CF, CG, CI,
CM, GA,	GN, GW, ML, MR, 1	NE, SN, TD, TG	
CA 2315717	AA 19990701	CA 1998-2315717	19981222
AU 9921989	A1 19990712	<u>AU 1999-21989</u>	19981222
		EP 1998-965981	
R: AT, BE,	CH, DE, DK, ES, F	FR, GB, GR, IT, LI, LU	, NL, SE, MC, PT,
IE, SI,	LT, LV, FI, RO		
TR 200002618	T2 20010420	TR 2000-20000261	319981222
JP 2001526220	T2 20011218	JP 2000-525 <u>097</u>	19981222
BR 9814374	A 20020514	BR 1998-14374	19981222
NO 2000003232	A 20000821	NO 2000-3232	
BG 104597	A 20010228	BG 2000-104597	
PRIORITY APPLN. INFO	).:	US 1997-996343 A	
		WO 1998-US26078 W	19981222
OTHER SOURCE(S):	MARPAT 131:73	3648	

AB A method for treatment of cancerous cell growth mediated by raf kinase comprises administration of urea derivs. ANHCONHB [I; A = substituted isoxazolyl, thienyl, thiadiazolyl, furyl, pyrazolyl, etc.; B = (substituted) mono-, di-, or tricyclic aryl, heteroaryl contg. ≥1 5-6 membered arom. structure contg. 0-4 N, O, or S atoms]. Reaction of 4-phenyloxyphenyl isocyanate with 5-amino-3-tert-butylisoxazole in methylene chloride and heating at reflux temp. for 2 days gave title

ΙΙ

compd. II. In an in vitro raf kinase assay, I displayed IC50 values of 1-10  $\mu \textrm{M}\,.$ 

## IT 135680-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 135680-03-4 HCAPLUS

CN Carbamic acid, [4-[(4-aminophenyl)methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 229002-05-5P

CN

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 229002-05-5 HCAPLUS

Urea, N-[4-[(4-aminophenyl)methyl]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

IT 229001-93-8P 229001-94-9P 229001-95-0P

 229001-96-1P
 229001-97-2P
 229001-98-3P

 229001-99-4P
 229002-00-0P
 229002-01-1P

 229002-02-2P
 229002-03-3P
 229002-04-4P

 229002-06-6P
 229002-07-7P
 229002-08-8P

 229002-12-4P
 229002-10-2P
 229002-11-3P

 229002-15-7P
 229002-16-8P
 229002-14-6P

 229002-15-7P
 229002-16-8P
 229002-17-9P

 229002-18-0P
 229002-19-1P
 229002-20-4P

 229002-21-5P
 229002-22-6P
 229002-23-7P

 229002-24-8P
 229002-25-9P
 229002-85-1P

 229002-86-2P
 229002-87-3P
 229002-97-5P

 229002-98-6P
 229002-99-7P
 229003-04-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 229001-93-8 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylmethoxy)phenyl]- (9C1) (CA INDEX NAME)

t-Bu

RN 229001-94-9 HCAPLUS

CN Benzamide, 5-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

t-Bu´

RN 229001-95-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[2-(4-pyridinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu´ RN

229001-96-1 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-methoxyphenyl)methylamino]phenyl]- (9CI) (CA INDEX NAME)

RN 2

229001-97-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

RN 229001-98-3 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN

229001-99-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[[2-(trifluoromethyl)-4-pyridinyl]thio]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-00-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)

RN 229002-01-1 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-hydroxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-02-2 HCAPLUS

CN Urea, N-[4-[(4-butoxyphenyl)thio]phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-03-3 HCAPLUS

CN Butanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN 229002-04-4 HCAPLUS

CN Carbamic acid, [4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 229002-06-6 HCAPLUS

CN Acetamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-07-7 HCAPLUS

CN Butanoic acid, 4-[[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

RN <u>229002-08-8</u> HCAPLUS

CN Propanamide, N-[4-[[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN

229002-09-9 HCAPLUS

 $\label{lem:urea} \mbox{ Urea, N-[4-(4-aminophenoxy)\,phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-1] } \mbox{ Proposition of the proposition of$ CN pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t.-Bui

229002-10-2 HCAPLUS

RN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-CN pyridinyloxy)phenyl] - (9CI) (CA INDEX NAME)

t-Bu

229002-11-3 HCAPLUS

RNCarbamic acid, [4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-CNyl]amino]carbonyl]amino]phenoxy]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

RN

229002-12-4 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-CN pyridinylmethyl)thio]phenyl] - (9CI) (CA INDEX NAME)

RN

229002-13-5 HCAPLUS

 $\label{lem:urea} \mbox{ Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-methylethyl)-1-methyl-1]-N'-[4-[(4-methylethyl)-1]-M'-[4-methylethyl]-N'-[4-methyl-1]-N'-[4-methylethyl]-N'-[4-methyl-1]-N'-[4-methylethyl]-N'-[4-methylethyl]-N'-[4-methyl-1]-N'-[4-methyl-1]-N'-[4-methyl-1]-N'-[4-methylethyl]-N'-[4-methyl-1]$ CN pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN

229002-14-6 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-(4-CN phenoxyphenyl) - (9CI) (CA INDEX NAME)

RN229002-15-7 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-CNpyridinylmethyl)phenyl] - (9CI) (CA INDEX NAME)

t-Bu

RN

CN

229002-16-8 HCAPLUS

 $\label{eq:Urea} \textit{Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-(4-x)]} = 0.$ methylphenoxy)phenyl] - (9CI) (CA INDEX NAME)

t-Bu

RN 229002-17-9 HCAPLUS

Urea, N-[3-(2-benzothiazolyloxy)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-CN1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN229002-18-0 HCAPLUS

 $\label{lem:urea} \textit{Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-pyrazol-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-yl]-N'-[4-[(4-phenyl-1)]-1-methyl-1-yl]-N'-[4-[(4-phenyl-1)]-N'-[4-[(4-phenyl-1)]-[4-[(4-p$ CN

2-thiazolyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 229002-19-1 HCAPLUS

CN Urea, N-[4-(2-benzothiazolylthio)-3-(trifluoromethyl)phenyl]-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-20-4 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-(1,1-dimethylethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-21-5 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[4-[4-[(trifluoromethyl)thio]phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-22-6 HCAPLUS

CN Urea, N-[1,1'-biphenyl]-3-yl-N'-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

RN 229002-23-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[3-

(phenylmethoxy)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-24-8 HCAPLUS

CN Butanamide, N-[4-[4-[[[[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]amino]carbonyl]amino]phenoxy]phenyl]-3-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{NH} - \text{C} - \text{NH} \\ \end{array}$$

t-Bu´

RN 229002-25-9 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[4-[(4-propoxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-26-0 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-(2,2,2-trifluoroethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu´ RN

229002-27-1 HCAPLUS

CN Urea, N-[1-(2-cyanoethyl)-3-(1,1-dimethylethyl)-1H-pyrazol-5-yl]-N'-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-28-2 HCAPLUS

CN 1H-Pyrazole-1-carboxylic acid, 3-(1,1-dimethylethyl)-5-[[[[4-[3-

[(methylamino)carbonyl]phenoxylphenyl]amino]carbonyl]amino]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 229002-85-1 HCAPLUS

CN Urea, N-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)-N'-[4-(6-quinolinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 229002-86-2 HCAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[4-[[[(1-methyl-3-phenyl-1H-pyrazol-5-yl)amino]carbonyl]amino]phenoxy]- (9CI) (CA INDEX NAME)

RN 229002-87-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[[(9H-fluoren-2-ylamino)carbonyl]amino]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 229002-97-5 HCAPLUS

CN Urea, N-(2,3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-(2-hydroxyethyl)-1+pyrazol-5-yl]- (9CI) (CA INDEX NAME)

t-Bu

RN 229002-98-6 HCAPLUS

CN 1H-Pyrazole-1-acetic acid, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

t-Buí

RN 229002-99-7 HCAPLUS

CN TH-Pyrazole-1-acetamide, 5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-N-methyl- (9CI) (CA INDEX NAME)

t-Bu RN

229003-04-7 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-methyl-1H-pyrazol-5-yl]-N'-[3-(4-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

IT 229003-22-9 229003-25-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; prepn. of substituted heterocyclic ureas for treatment of cancerous cell growth mediated by raf kinase)

RN 229003-22-9 HCAPLUS

Carbamic acid, (2,3-dichlorophenyl)-, 2-[5-[[[(2,3-dichlorophenyl)amino]carbonyl]amino]-3-(1,1-dimethylethyl)-1H-pyrazol-1-yl]ethyl ester (9CI) (CA INDEX NAME)

229003-25-2 HCAPLUS RN

CNCarbamic acid, [4-[4-[[[[5-(1,1-dimethylethyl)-3isoxazolyl]amino]carbonyl]amino]phenoxy]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

7

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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# References

ACCESSION NUMBER:

DOCUMENT NUMBER:

INVENTOR(S):

TITLE:

1998:402427 HCAPLUS

129:81759

Preparation and formulation of benzodiazepine

derivatives as gastrin and cholecystokinin antagonists

Shinozaki, Katsuo; Yoneta, Tomoyuki; Murata, Masakazu;

Miura, Naoyoshi; Maeda, Kiyoto

PATENT ASSIGNEE(S):

Zeria Pharmaceutical Co., Ltd., Japan; Shinozaki, Katsuo;; Yoneta, Tomoyuki;; Murata Masakazu;; Miura,

Naoyoshi;; Maeda, Kiyoto;

PCT Int. Appl., 432 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		KIND	DATE		APPLICA	ATION NO.	DATE			
WO 9825911	<b>=</b> .	A1	19980618		WO 199	7-JP4534	19971210			
W: AU	J, CA,	CN, JP	, KR, US							
RW: AT	BE,	CH, DE	, DK, ES,	FΙ,	FR, GB, G	GR, IE, I	T, LU, MC,	NL,	PT,	SE
AU 9854100	)	A1	19980703		AU 1998	8-54100	19971210			
AU 721081		B2	20000622							
EP 945445		A1	19990929		EP 199'	7-947872	19971210			

EP 945445	В1	20030903		
R: AT, BE, C	H, DE	, DK, ES,	FR, GB, GR, IT, LI, LU	, NL, SE, MC, PT,
IE, FI				
CN 1246850	A	20000308	CN 1997-181599	19971210
CN 1130351	В	20031210		
AT 248823	E	20030915	AT 1997-947872	19971210
PT 945445	$\mathbf{T}$	20040130	PT 1997-947872	19971210
ES 2206754	Т3	20040516	ES 1997-947872	19971210
US 6239131	B1	20010529	US 1999-319249	19990608
KR 2000057506	A	20000915	KR 1999-705193	19990610
PRIORITY APPLN. INFO.:			JP 1996-344498 A	19961210
101.101.001.001			JP 1997-156132 A	19970530
			WO 1997-JP4534 W	19971210
		DDIE 100	34850	

OTHER SOURCE(S):

MARPAT 129:81759

Ι

GΙ

$$\begin{array}{c} \text{(CH 2)}_{n-R^2} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{NH CO NH} \\ \text{Ar} \\ \text{R5} \\ \end{array}$$

Me 
$$CO - CH_2 O$$
  $N - NH CO NH$   $CO_2H$   $CO_2$ 

The title compds. I [R1 represents hydrogen, lower alkyl, lower alkoxy or halogeno; R2 and R3 may be the same or different and each represents hydrogen, alkenyl, alkyl, Ph, acyl, etc.; and R4 and R5 may be the same or different and each represents hydrogen, alkyl, carboxyl, etc.; Ar = arom. heterocycle, etc.; n = 0 or 2] are prepd. The compds. have an excellent gastrin and/or CCK-B receptor antagonism and are useful as remedies for gastric ulcer and gastrointestinal movement disorder. In an in vitro test for CCK-B receptor antagonism, the title compd. (+)-II showed the Ki value of 1.16 nM. (+)-II at 1 mg/kg intraduodenally gave 81% inhibition of stomach acid secretion induced by pentagastrin 15 μg/kg/h in rats.

IT 209219-48-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN <u>209219-48-7</u> HCAPLUS

CN Urea, N-[5-cyclohexyl-1-(3,3-dimethyl-2-oxobutyl)-2,3,4,5-tetrahydro-2-oxo-1H-1,5-benzodiazepin-3-yl]-N'-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

IT 19962-06-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN <u>19962-06-2</u> HCAPLUS

CN Carbamic acid, (3-hydroxyphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 209222-94-6P 209222-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of benzodiazepine derivs. as gastrin and cholecystokinin antagonists)

RN 209222-94-6 HCAPLUS

CN Propanoic acid, 2-[3-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 209222-95-7 HCAPLUS

CN Propanoic acid, 2-[3-[[(1,1-dimethylethoxy)carbonyl]amino]phenoxy]-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

1995:709095 HCAPLUS

DOCUMENT NUMBER: 123:218414

TITLE:

Imidazoles and antiarteriosclerotics containing the

imidazoles

INVENTOR(S):

Kumazawa, Toshiaki; Harakawa, Hiroyuki; Fukui, Hiromi;

Shirokura, Shiro; Ooishi, Eiko; Yamada, Koji

PATENT ASSIGNEE(S):

SOURCE:

Kyowa Hakko Kogyo Kk, Japan

Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

KIND DATE APPLICATION NO.

DATE

JP 07133224

A2

19950523 JP 1993-280961 19931110

PRIORITY APPLN. INFO.:

JP 1993-280961

OTHER SOURCE(S):

MARPAT 123:218414

Antiarteriosclerotics contain imidazoles I [X, Y = CH, N; Z = single bond, AΒ CH2; R1, R2, R3 = H, halo, lower alkyl, OH, lower alkoxy, carboxy, lower alkoxycarbonyl, NH2, mono- or di-lower alkyl-substituted amino, carbamoyl, mono- or di-lower alkyl-substituted carbamoyl, CF3; R4, R5, R6 = H, halo, lower alkyl, lower alkoxy; R7 = H, lower alkyl, lower alkyl-(un) substituted cycloalkyl] or their pharmacol. acceptable salts as active ingredients. N-[1-(2-chlorophenyl)-2-benzimidazolyl]-N'-(2,6diisopropylphenyl)urea (II) (2.3 g) was prepd. by treatment of 1.5 g 2-amino-1-(2-chlorophenyl)benzimidazole and 1.46 mL 2,6-diisopropylphenyl isocyanate. II (at 10-7M) inhibited acyl CoA: cholesterol acyltransferase by 85%. II showed min. LD of >100 mg/kg i.p. in mice. A formulation example of tablets is given.

IT 168120-11-4P 168120-12-5P 168120-13-6P

168120-16-9P 168120-18-1P 168120-21-6P

168120-32-9P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN168120-11-4 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-(1-phenyl-1H-benzimidazol-2-yl)-(9CI) (CA INDEX NAME)

RN <u>168120-12-5</u> HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-13-6 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(3-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-16-9 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-methylphenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-18-1 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-(dimethylamino)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN168120-21-6 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2,6-dichlorophenyl)-1H-CNbenzimidazol-2-yl]- (9CI) (CA INDEX NAME)

168120-32-9 HCAPLUS RN

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[3-(2-chlorophenyl)-3H-CNimidazo[4,5-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)

IT 168120-19-2P 168120-27-2P 168120-30-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN 168120-19-2 HCAPLUS

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-methoxyphenyl)-1H-CNbenzimidazol-2-yl]- (9CI) (CA INDEX NAME)

168120-27-2 HCAPLUS

Benzoic acid, 3-[2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]-CN1H-benzimidazol-1-yl]-4-chloro-, methyl ester (9CI) (CA INDEX NAME)

RN 168120-30-7 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-6-methoxy-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

IT 168120-14-7P 168120-15-8P 168120-17-0P

168120-20-5P 168120-22-7P 168120-23-8P

168120-24-9P 168120-25-0P 168120-26-1P

168120-28-3P 168120-29-4P 168120-31-8P

168120-33-0P 168120-34-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiarteriosclerotics contg. imidazoles)

RN 168120-14-7 HCAPLUS

CN

Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-chlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-15-8 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-bromophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-17-0 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-(trifluoromethyl)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-20-5 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-hydroxyphenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-22-7 HCAPLUS

CN Urea, N-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,4-difluorophenyl)(9CI) (CA INDEX NAME)

RN 168120-23-8 HCAPLUS

CN Urea, N-[1-(2-chlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,6-dimethylphenyl)-(9CI) (CA INDEX NAME)

RN 168120-24-9 HCAPLUS

CN Urea, N-[1-(2,6-dichlorophenyl)-1H-benzimidazol-2-yl]-N'-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

RN 168120-25-0 HCAPLUS

CN Urea, N-(2,6-dichlorophenyl)-N'-[1-(2,6-dichlorophenyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 168120-26-1 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-[2-chloro-4-(dimethylamino)phenyl]-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-28-3 HCAPLUS

CN Benzoic acid, 3-[2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]-1H-benzimidazol-1-yl]-4-chloro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{i-Pr} \\ \text{NH} - \text{C-NH} \\ \text{i-Pr} \\ \text{HO } 2\text{C} \\ \end{array}$$

RN 168120-29-4 HCAPLUS

CN 1H-Benzimidazole-6-carboxylic acid, 2-[[[[2,6-bis(1-methylethyl)phenyl]amino]carbonyl]amino]-1-(2-chlorophenyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & i\text{-Pr} \\ 0 \\ 0 \\ 0 \\ \end{array}$$

RN 168120-31-8 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(2-chlorophenyl)-6-hydroxy-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-33-0 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-chloro-3-pyridinyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

RN 168120-34-1 HCAPLUS

CN Urea, N-[2,6-bis(1-methylethyl)phenyl]-N'-[1-(4-methyl-2-pyridinyl)-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

IT 138046-81-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction in prepn. of imidazoles as antiarteriosclerotics)

RN 138046-81-8 HCAPLUS

CN Carbamic acid, (2,4,6-trimethylphenyl)-, phenyl ester (9CI) (CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 106.97 692.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

-14.55
-16.53

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter  $\frac{\text{HELP FIRST}}{\text{FORMULE}}$  for more information.

#### => d his

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

L8 50 S L7

L9 1575 S L7 FULL

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004 L10 225 S L9/PREP

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FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
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L12
             50 S L11
T.13
                STRUCTURE UPLOADED
T.14
             49 S L13
T.15
                STRUCTURE UPLOADED
L16
              8 S L15
L17
                STRUCTURE UPLOADED
L18
             50 S L17
                E INDANYL/CN
L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
              1 S E3
T.2.1
L22
                STRUCTURE UPLOADED
L23
             50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
T<sub>1</sub>2.5
           6528 S L24/RCT
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
               STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
              0 S L26 AND TAN, Z?/AU
L30
              0 S L26 AND SONG, J?/AU
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
=> s 124 and 19
TOO MANY TERMS FOR FILE CROSSOVER IN L24
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.
=> s 19
            14 L9
T.31
=> s 124
TOO MANY TERMS FOR FILE CROSSOVER IN L24
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.
=> file reg
COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                 TOTAL
                                                       ENTRY
                                                              SESSION
FULL ESTIMATED COST
                                                        2.10
                                                                694.23
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                SINCE FILE
                                                                 TOTAL
                                                      ENTRY
                                                                SESSION
CA SUBSCRIBER PRICE
                                                        0.00
                                                                -16.53
FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

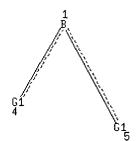
Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

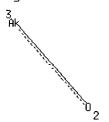
Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e 2-amino pyrazole/cn
E1
                    2-AMINO CYCLIC AMP/CN
E2
                    2-AMINO MUSK XYLENE/CN
E3
              0 --> 2-AMINO PYRAZOLE/CN
                    2-AMINO ((METHOXYCARBONYL) THIOUREIDO) BENZENE/CN
E4
E5
             1
                    2-AMINO(1)BENZOTHIENO(2,3-B)(1)BENZOTHIOPYRAN-11-ONE/CN
E6
              1
                    2-AMINO (HYDRAZONO) METHYL-1, 10-PHENANTHROLINE/CN
F.7
                    2-AMINO (PENTAFLUOROETHYL) BENZENE HYDROCHLORIDE/CN
             1
E8
                    2-AMINO-(3-(TERT-BUTYLOXYCARBONYL)PIPERIDIN-1-YL)BENZENE/CN
             1
F.9
                    2-AMINO-.ALPHA.,.ALPHA.,.S,6-PENTAFLUOROACETOPHENONE/
             1
E10
             1
                    2-AMINO-.ALPHA.,.ALPHA.,.ALPHA.-TRIFLUORO-P-TOLUENESULFONAMI
                   DE/CN
E11
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             1
                    CHLORIDE/CN
E12
             1
                    2-AMINO-.ALPHA.,.ALPHA.,.ALPHA.-TRIFLUOROTOLUENE/CN
=> e amino pyrazole/cn
            1
                   AMINO PEGA RESIN/CN
E2
                   AMINO POLYOL AMINE OXIDASE/CN
E3
             0 --> AMINO PYRAZOLE/CN
E4
                  AMINO RADICAL/CN
                  AMINO RADICAL (NH2)/CN
E5
E6
             1
                  AMINO SEPHAROSE 6 FAST FLOW/CN
E.7
             1
                  AMINO SILOXANES AND SILICONES/CN
E.8
                  AMINO TRANSFERASE (STREPTOMYCES COELICOLOR STRAIN A3(2) GENE
             1
                   SCF55.27)/CN
E9
             1
                   AMINO TRANSFERASE (THERMUS THERMOPHILUS STRAIN HB8)/CN
E10
             1
                   AMINO VALERIC ACID/CN
E11
             1
                   AMINO (((2-NITROPHENYL) METHYL) AMINO) METHANE-1-THIONE/CN
E12
                   AMINO ((3,4-DICHLOROPHENYL) AMINO) METHANE-1-THIONE/CN
=>
L32
        STRUCTURE UPLOADED
=> d 132
L32 HAS NO ANSWERS
L32
                STR
Ak & 0 M1 X 8
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Page 1-A



Page 1-B



Page 2-B VAR G1=6/7/8/2

NODE ATTRIBUTES:

HCOUNT IS M1 ATIS C NSPEC ATIS C NSPEC ATIS C NSPEC AT3 NSPEC IS C AT4 NSPEC IS C AT

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 2 3 6 7 8

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

=> s 132

SAMPLE SEARCH INITIATED 10:23:58 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 16360 TO ITERATE

6.1% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

319545 TO 334855

PROJECTED ANSWERS:

79883 TO 87643

L33

50 SEA SSS SAM L32

=> s 132 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y FULL SEARCH INITIATED 10:24:12 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 327382 TO ITERATE

50 ANSWERS

100.0% PROCESSED 327382 ITERATIONS SEARCH TIME: 00.00.04

89725 ANSWERS

L34 89725 SEA SSS FUL L32

=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST

ENTRY SESSION 159.20 853.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

CA SUBSCRIBER PRICE

ENTRY SESSION 0.00 -16.53

FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
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FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26 FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 134/rct

117519 L34

2633407 RCT/RL

L35 36779 L34/RCT

(L34 (L) RCT/RL)

=> d his

L7

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 STRUCTURE UPLOADED

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FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
 L8
             50 S L7
 L9
            1575 S L7 FULL
      FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
 L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
 L11
                STRUCTURE UPLOADED
 L12
             50 S L11
 L13
                STRUCTURE UPLOADED
             49 S L13
L14
L15
                STRUCTURE UPLOADED
              8 S L15
L16
L17
                STRUCTURE UPLOADED
L18
             50 S L17
                E INDANYL/CN
L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
L24
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
               STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
              0 S L26 AND TAN, Z?/AU
L29
L30
              0 S L26 AND SONG, J?/AU
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
            14 S L9
     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
               E 2-AMINO PYRAZOLE/CN
                E AMINO PYRAZOLE/CN
L32
                STRUCTURE UPLOADED
L33
             50 S L32
         89725 S L32 FULL
     FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
L35
          36779 S L34/RCT
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     FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
     FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
Ll
                STRUCTURE UPLOADED
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0 S L1
L3
               0 S L1 FULL
L4
                 STRUCTURE UPLOADED
L5
               0 S L4
L6
               3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7
                 STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
L8
             50 S L7
L9
           1575 S L7 FULL
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                STRUCTURE UPLOADED
L12
             50 S L11
L13
                STRUCTURE UPLOADED
L14
             49 S L13
L15
                STRUCTURE UPLOADED
L16
              8 S L15
L17
                STRUCTURE UPLOADED
L18
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L19
              1 S E7
                E BENZOFURAN/CN
L20
              1 S E3
                E INDENYL/CN
              1 S E3
T<sub>1</sub>2.1
L22
                STRUCTURE UPLOADED
L23
             50 S L22
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
L26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                STRUCTURE UPLOADED
L28
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     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
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L30
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     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
             14 S L9
     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
                E 2-AMINO PYRAZOLE/CN
                E AMINO PYRAZOLE/CN
L32
                STRUCTURE UPLOADED
L33
             50 S L32
L34
          89725 S L32 FULL
     FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004
L35
          36779 S L34/RCT
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=> d his
      (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
     FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
     FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
L1
                STRUCTURE UPLOADED
L2
               0 S L1
L3
               0 S L1 FULL
L4
                STRUCTURE UPLOADED
L5
               0 S L4
L6
              3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7
                STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
L8
             50 S L7
L9
           1575 S L7 FULL
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                STRUCTURE UPLOADED
L12
             50 S L11
L13
                STRUCTURE UPLOADED
L14
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L15
                STRUCTURE UPLOADED
L16
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L17
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L18
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L19
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                E BENZOFURAN/CN
L20
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                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
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L24
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     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
L26
            21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
              0 S L26 AND TAN, Z?/AU
L29
              0 S L26 AND SONG, J?/AU
L30
     FILE 'CAOLD' ENTERED AT 10:15:20 ON 24 JUN 2004
L31
             14 S L9
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FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004

E 2-AMINO PYRAZOLE/CN

E AMINO PYRAZOLE/CN L32 STRUCTURE UPLOADED L33 50 S L32 L34 89725 S L32 FULL

FILE 'HCAPLUS' ENTERED AT 10:24:24 ON 24 JUN 2004 L35 36779 S L34/RCT

=> s 135 and 126

L36 1 L35 AND L26

=> d 136, ibib abs, 1

L36 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2000:666713 HCAPLUS

DOCUMENT NUMBER: 133:252426

TITLE: Preparation of aromatic heterocyclic ureas as

antiinflammatory agents

INVENTOR(S): Betageri, Rajashehar; Breitfelder, Steffen; Cirillo,

Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.; Kirrane, Thomas M.; Moriak, Monica H.; Moss, Neil; Patel, Usha R.; Proudfoot, John R.; Regan, John R.;

Sharma, Rajiv; Sun, Sanxing; Swinamer, Alan D.;

Takahashi, Hidenori

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA SOURCE:

PCT Int. Appl., 282 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent LANGUAGE . English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE		APPLICATION NO. DATE
WO 2000055139	A2 200009	21	WO 2000-US3865 20000216
WO 2000055139			
W: AE, AU,	BG, BR, BY, C	A, CN,	CZ, EE, HR, HU, ID, IL, IN, JP, KR,
			RO, RU, SG, SI, SK, TR, UA, UZ, VN,
YU, ZA		•	, 1, 11, 11, 11, 11, 11, 11,
RW: AT, BE,	CH, CY, DE, D	K, ES.	FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE	, , ,	. ,	. , , , , , , , , , , , , , , , , , , ,
EP 1165516	A2 200201	02	EP 2000-907295 20000216
			GB, GR, IT, LI, LU, NL, SE, MC, PT,
	LT, LV, FI, R		, , , ==, ==, ==, ==, ==, ==,
			BR 2000-8922 20000216
			TR 2001-20010281720000216
			JP 2000-605569 20000216
			EE 2001-483 20000216
NZ 514711	A 200402	27	NZ 2000-514711 20000216
AU 771273			AU 2000-28817 20000216
		31	BG 2001-105880 20010905
ZA 2001007446			ZA 2001-7446 20010910
HR 2001000665			HR 2001-665 20010910
NO 2001004412			NO 2001-4412 20010911
US 2002055507			US 2001-962709 20010925
US 6660732			
		27	US 2001-962057 20010925
US 6656933			

US 2003225077 A1 20031204 US 2003-424613 20030428 US 2004019038 A1 20040129 US 2003-624289 20030721 PRIORITY APPLN. INFO.: US 1999-124148P P 19990312 US 1999-165867P P 19991116 US 2000-505582 A3 20000216 WO 2000-US3865 W 20000216 US 2001-962057 A1 20010925 US 2001-962709 A3 20010925

MARPAT 133:252426

ΙI

OTHER SOURCE(S):

GI

AΒ The title compds. (I) [wherein Ar1 = (un) substituted pyrrole, pyrrolidine, pyrazole, imidazole, oxazole, thiazole, furan, or thiophene; Ar2 = (un) substituted Ph, (tetrahydro) naphthyl, (tetrahydro) quinoline, (tetrahydro)isoquinoline, benzimidazole, benzofuran, indanyl, indenyl, or indole; W = O or S; X = (un) substituted cycloalkyl, cycloalkenyl, Ph, furan, thiophene, pyrrole, imidazolyl, pyridine, pyrimidine, (dihydro)pyridinone, (dihydro)maleimide, piperidine, piperazine, or pyrazine; Y = a bond or (un) substituted satd. or unsatd. alkyl optionally interrupted by O, NH, S(O), SO2, or S; Z = (un) substituted Ph, pyridine, pyrimidine, pyridazine, imidazole, (tetrahydro)furan, thiophene, (tetrahydro)pyran, 1,3-dioxolanone, 1,3-dioxanone, 1,4-dioxane, (thio) morpholine (sulfoxide), piperidine, cyclohexanone, pentamethylene sulfoxide, etc.] were prepd. for the treatment of diseases or pathol. conditions involving inflammation, such as chronic inflammatory diseases. Thus, coupling 2-cyclohexenone with 4-bromo-1-naphthylamine in the presence of Pd(PPh3)2Cl2, DPPP, and NaHCO3 in DMF, followed by conversion of the amine to an isocyanate using ClCOCl and immediate addn. of 1-(4-methylphenyl)-3-tert-butyl-1H-pyrazol-5-amine, gave the urea II. a cytokine prodn. inhibition assay, preferred compds. of the invention showed IC50 < 10  $\mu$ M against TNF- $\alpha$  in lipopolysaccharide stimulated THF cells.

=> file caold COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 16.70 870.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

-0.69

-17.22

FILE 'CAOLD' ENTERED AT 10:28:13 ON 24 JUN 2004
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REG1STRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

#### => d his

1.4

(FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004

FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

STRUCTURE UPLOADED

L5 0 S L4

L6 3 S L4 FULL

FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004 L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004

L8 50 S L7

L9 1575 S L7 FULL

FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004 L10 225 S L9/PREP

FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004

L11 STRUCTURE UPLOADED

L12 50 S L11

L13 STRUCTURE UPLOADED

L14 49 S L13

L15 STRUCTURE UPLOADED

L16 8 S L15

L17 STRUCTURE UPLOADED

L18 50 S L17

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E BENZOFURAN/CN

L20 1 S E3

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E INDENYL/CN
1.21
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L22
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L23
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L24
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            6528 S L24/RCT
L26
              21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                 STRUCTURE UPLOADED
L28
              50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
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L30
               0 S L26 AND SONG, J?/AU
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     FILE 'REGISTRY' ENTERED AT 10:18:16 ON 24 JUN 2004
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L32
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L33
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L35
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     FILE 'CAOLD' ENTERED AT 10:28:13 ON 24 JUN 2004
=> s 134 and 19
TOO MANY TERMS FOR FILE CROSSOVER IN L34
There are limits on the size of an answer set being crossed over from
one file to another. Enter <a href="https://example.com/HELP_CROSSOVER">HELP_CROSSOVER</a> at an arrow prompt (=>)
for specific information.
=> s 19 and 134
TOO MANY TERMS FOR FILE CROSSOVER IN L34
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.
=> s 131 and base
          9375 BASE
          6467 BASES
         15700 BASE
                  (BASE OR BASES)
L37
             0 L31 AND BASE
=> file reg
COST IN U.S. DOLLARS
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                                                                    TOTAL
                                                        ENTRY
                                                                 SESSION
FULL ESTIMATED COST
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
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                                                        ENTRY
                                                                  SESSION
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

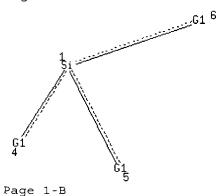
Crossover limits have been increased. See <a href="HELP CROSSOVER">HELP CROSSOVER</a> for details.

Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> L38 STRUCTURE UPLOADED

=> d 138 L38 HAS NO ANSWERS L38 STR

Ak 80 M1 X 9 Page 1-A





Page 2-B VAR G1=7/8/9/2 NODE ATTRIBUTES: HCOUNT IS M1

AT 8

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AT
NSPEC IS C
                      AT
NSPEC
         IS C
                      AT
NSPEC
         IS C
                      AΤ
                            5
                     AT
NSPEC IS C
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 1 2 3 7 8 9
DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
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SAMPLE SEARCH INITIATED 10:35:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 55513 TO ITERATE
  1.8% PROCESSED
                        1000 ITERATIONS
                                                                             50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
                            BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS:
                                EXCEEDS 584795
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              1
E2
                1
                       SILICOMONAZITE/CN
EЗ
               1 --> SILICON/CN
            1 --> SILICON/CN

1 SILICON (DIPHOSPHATE)/CN

1 SILICON (SI(3+))/CN

1 SILICON (SI10+) CLUSTER ION/CN

1 SILICON (SI11+) CLUSTER ION/CN

1 SILICON (SI12+) CLUSTER ION/CN

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1 SILICON (SI16+) CLUSTER ION/CN
E4
E5
E6
E7
E8
E9
E10
E11
E12
=> s e3
L40
               1 SILICON/CN
=> d 13
L3 HAS NO ANSWERS
L3
               0 SEA FILE=CASREACT SSS FUL L1 ( 0 REACTIONS)
=> d his
      (FILE 'HOME' ENTERED AT 09:29:11 ON 24 JUN 2004)
      FILE 'REGISTRY' ENTERED AT 09:29:19 ON 24 JUN 2004
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FILE 'CASREACT' ENTERED AT 09:43:31 ON 24 JUN 2004
 L1
                 STRUCTURE UPLOADED
 L_2
               0 S L1
 L3
               0 S L1 FULL
 L4
                 STRUCTURE UPLOADED
 L5
               0 S L4
 L6
               3 S L4 FULL
     FILE 'REGISTRY' ENTERED AT 09:47:01 ON 24 JUN 2004
L7
                 STRUCTURE UPLOADED
     FILE 'REGISTRY' ENTERED AT 09:48:17 ON 24 JUN 2004
L8
              50 S L7
            1575 S L7 FULL
L9
     FILE 'HCAPLUS' ENTERED AT 09:48:40 ON 24 JUN 2004
L10
            225 S L9/PREP
     FILE 'REGISTRY' ENTERED AT 09:48:47 ON 24 JUN 2004
L11
                 STRUCTURE UPLOADED
L12
              50 S L11
L13
                STRUCTURE UPLOADED
L14
             49 S L13
L15
                STRUCTURE UPLOADED
L16
              8 S L15
L17
                STRUCTURE UPLOADED
L18
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                E INDANYL/CN
L19
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                E BENZOFURAN/CN
L20
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                E INDENYL/CN
L21
              1 S E3
L22
                STRUCTURE UPLOADED
L23
             50 S L22
          65845 S L22 FULL
     FILE 'HCAPLUS' ENTERED AT 10:10:57 ON 24 JUN 2004
L25
           6528 S L24/RCT
1,26
             21 S L25 AND L10
     FILE 'REGISTRY' ENTERED AT 10:13:07 ON 24 JUN 2004
L27
                STRUCTURE UPLOADED
L28
             50 S L27
     FILE 'HCAPLUS' ENTERED AT 10:13:28 ON 24 JUN 2004
L29
           0 S L26 AND TAN, Z?/AU
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L31
             14 S L9
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                E AMINO PYRAZOLE/CN
L32
                STRUCTURE UPLOADED
L33
             50 S L32
L34
          89725 S L32 FULL
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# **Patent Assignment Abstract of Title**

Total Assignments: 1

**Application #:** 10074895 Filing Dt: 02/12/2002

Patent #: NONE

Issue Dt:

PCT #: NONE

Publication #: <u>US20020123631</u> Pub Dt: 09/05/

Inventors: Zhulin Tan, Jinhua J. Song

Title: Process for synthesis of heteroaryl-substituted urea compounds useful as

antiinflammatory agents

Assignment: 1

Reel/Frame: 012594/0147 Received: 02/26/2002 Recorded: 02/12/2002 Mailed: 04/17/2002 Pag

Conveyance: ASSIGNMENT OF ASSIGNORS INTEREST (SEE DOCUMENT FOR DETAILS).

Assignors: TAN, ZHULIN

Exec Dt: 01/17/2002

SONG, JINHUA J.

Exec Dt: 01/17/2002

Assignee: BOEHRINGER INGELHEIM PHARMACEUTICALS, INC.

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Search Results as of: 6/20/2004 10:47:05 P.M.